CAS ONLINE PRINTOUT

=> d his

(FILE 'HOME' ENTERED AT 07:36:41 ON 18 OCT 2007)

FILE 'CASREACT' ENTERED AT 07:37:09 ON 18 OCT 2007
L1 STRUCTURE UPLOADED
L2 17 S L1
L3 0 S FCRDREF
L4 628 S L1 FUL
L5 26908 S PALLADIUM
L6 68 S L5 AND L4

FILE 'REGISTRY' ENTERED AT 07:41:31 ON 18 OCT 2007
E CARBON DIOXIDE/CN
L7 1 S E3

FILE 'CASREACT' ENTERED AT 07:41:56 ON 18 OCT 2007
L8 5511 S L7
L9 4 S L8 AND L6

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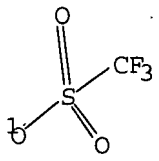

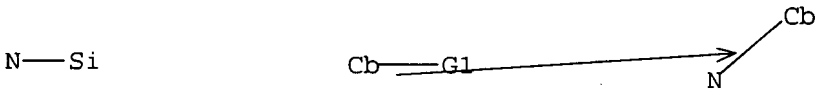

G1 X,[@1]

Structure attributes must be viewed using STN Express query preparation.

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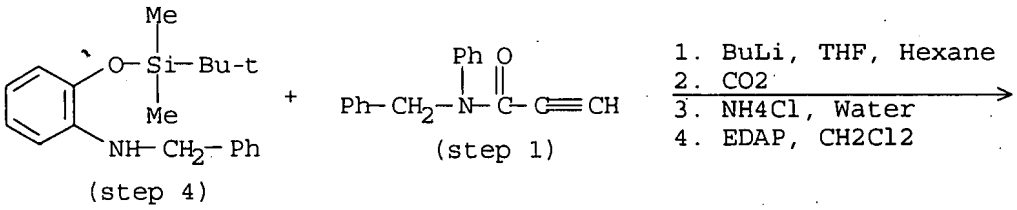
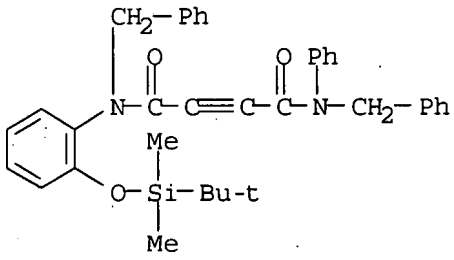
L9 ANSWER 1 OF 4 CASREACT COPYRIGHT 2007 ACS on STN

CAS ONLINE PRINTOUT

RX(25) OF 241

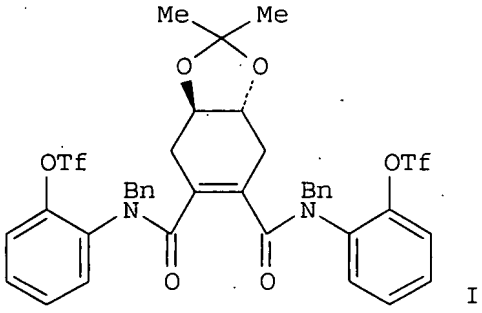




32%

REF: Journal of Organic Chemistry, 71(7), 2587-2599; 2006
CON: STAGE(1) 0.5 hours, -78 deg C
STAGE(2) 5 minutes, -78 deg C; -78 deg C -> room temperature
STAGE(4) -60 deg C; 2 hours, -60 deg C -> -5 deg C

AN 144:350197 CASREACT
TI Diastereoselection in the formation of spirocyclic oxindoles by the intramolecular Heck reaction
AU Overman, Larry E.; Watson, Donald A.
CS Department of Chemistry, University of California, Irvine, CA, 92697-2025, USA
SO Journal of Organic Chemistry (2006), 71(7), 2587-2599
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
GI



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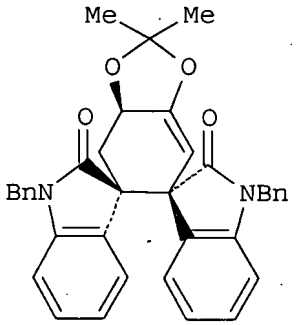


II

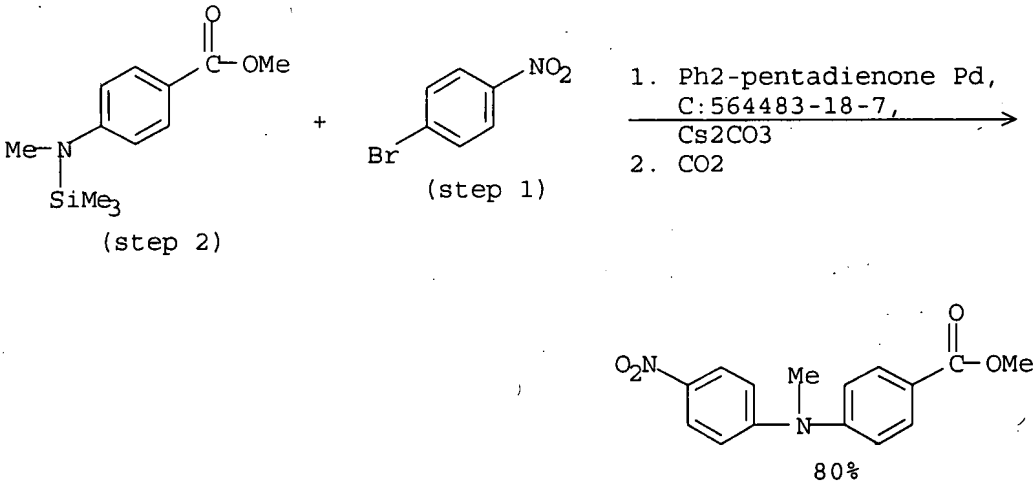
AB Diastereoselective double Heck cyclizations of cyclohexene diamides [e.g., trans-acetonide 1 (I) and its trans-disiloxy analog 3] form contiguous quaternary stereocenters (e.g., II from I), with diastereoselection being controlled by the trans-diol protecting group. In this, the first in a series of two papers, the origin of diastereoselection in the first ring-closure step of these reactions is examined Nine simplified analogs of 1 and 3 were synthesized and cyclized to discern what structural features are required to realize high diastereoselection in the first intramol. Heck reaction. These studies show that high stereoselection (>20:1) does not arise from a single structural feature: it is seen only in substrates that contain both a trans-acetonide and a tertiary amide substituent at C2. Two subtle factors appear to be involved: avoidance of eclipsing interactions between the forming C-C bond and the pseudoaxial hydrogen atom at C6 and between the pseudoequatorial hydrogen atom at C6 and the carbonyl carbon of the forming spirooxindole. The vinylic amide substituent that is not involved in the insertion event preferentially adopts a perpendicular conformation, placing the sterically bulky NR2 over the alkene π bond. Syn-Pentane-like interactions between this substituent and the C3 of the cyclohexene are avoided in the favored insertion topog. These two effects, when combined, produce a highly diastereoselective process. Safety was recommend use of glass-lined steel reactor for preparation of diacid chloride intermediates for Heck cyclization substrates via Diels-Alder reaction.

RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 4 CASREACT COPYRIGHT 2007 ACS on STN

CAS ONLINE PRINTOUT

RX(4) OF 73



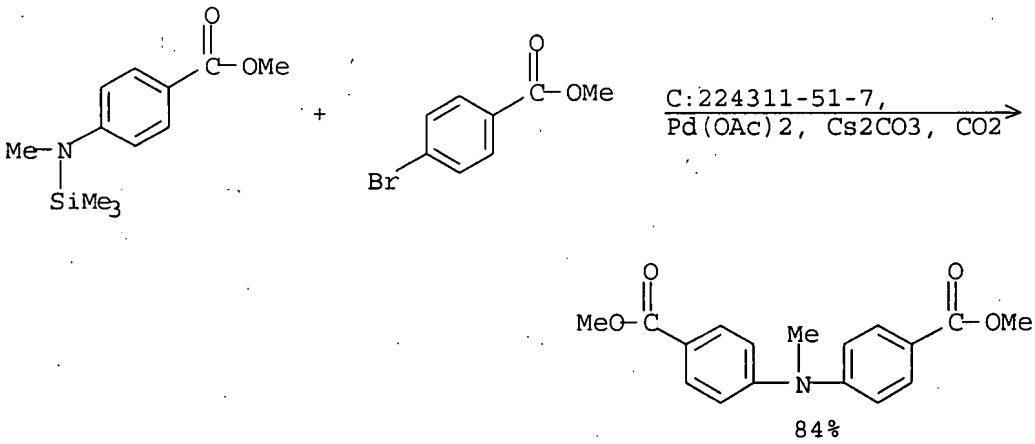
REF: Organic & Biomolecular Chemistry, 3(20), 3767-3781; 2005
NOTE: supercritical, green chemistry - solvent, high pressure in second stage, reaction in a sealed high pressure cell, incremental addition of solvent in second stage
CON: STAGE(1) room temperature
STAGE(2) 800 psi; 100 deg C, 800 psi; 800 psi -> 1800 psi; 17 hours, 100 deg C, 1800 psi; 100 deg C -> room temperature

AN 144:6541 CASREACT
TI Palladium catalyzed aryl amination reactions in supercritical carbon dioxide
AU Smith, Catherine J.; Tsang, Melanie W. S.; Holmes, Andrew B.; Danheiser, Rick L.; Tester, Jefferson W.
CS Department of Chemistry, Melville Laboratory, Cambridge, CB2 1EW, UK
SO Organic & Biomolecular Chemistry (2005), 3(20), 3767-3781
CODEN: OBCRAK; ISSN: 1477-0520
PB Royal Society of Chemistry
DT Journal
LA English
AB Palladium catalyzed C-N bond formation in supercrit. carbon dioxide has been accomplished. Carbamic acid formation is avoided in part through the use of an N-silylamine as the coupling partner. Employing a catalyst system of Pd2dba3 (1 mol%) and 2-dicyclohexylphosphino-2',4',6'-triisopropyl-1,1'-biphenyl (X-Phos) (2 mol%) enabled the catalytic amination of aryl bromides and chlorides with N-silylanilines to be realized in excellent yield. Extension of the methodol. to the N-arylation of N-silyldiarylamines, N-silylazoles and N-silylsulfonamides is reported.
RE.CNT 72 THERE ARE 72 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 3 OF 4 CASREACT COPYRIGHT 2007 ACS on STN

CAS ONLINE PRINTOUT

RX(1) OF 24



REF: PCT Int. Appl., 2005090283, 29 Sep 2005
NOTE: high pressure, yield depends on reaction pressure, supercritical CO2 used as solvent
CON: 17 hours, 100 deg C, 3000 psi

AN 143:306029 CASREACT
TI Amination of aromatic compounds using transition metal catalysts
IN Holmes, Andrew Bruce; Smith, Catherine Janet; Tsang, Melanie Wing-Sze; Early, Theresa Rachel; Shute, Richard Eden
PA Cambridge University Technical Services Limited, UK; Astrazeneca UK Limited
SO PCT Int. Appl., 41 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005090283	A1	20050929	WO 2005-GB1130	20050318
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	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	EP 1737812	A1	20070103	EP 2005-718110	20050318
	R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
	US 2007179315	A1	20070802	US 2007-593212	20070223
PRAI	GB 2004-6125		20040318		
	WO 2005-GB1130		20050318		

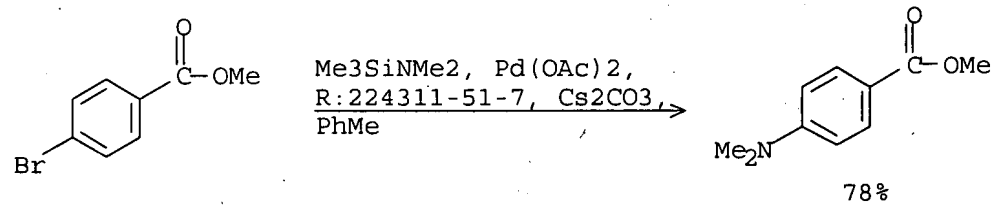
OS MARPAT 143:306029
AB A method for synthesizing amines R1NR2R3 (R1 is optionally substituted aryl; R2 is optionally substituted aryl, heterocyclyl, alkyl or sulfonyl; R3 is H or optionally substituted alkyl, heterocyclyl or aryl; or R2R3N is optionally substituted heterocyclyl or heteroaryl) comprises reacting R1-L, where L is a labile leaving group, with a silylamine R2R3NSiR4R5R6 (R4, R5, R6 are independently optionally substituted alkyl, aryl,

heterocyclyl, hydroxy, halo, amino or alkoxy or two of R1, R2 and R3, together with the silicon atom may form a ring) in compressed carbon dioxide in the presence of a transition metal catalyst and a base. Thus, a stainless steel cell containing Me p-bromobenzoate, Cs2CO3, palladium acetate, and di-tert-butylbiphenylphosphine was evacuated and refilled with nitrogen, p-MeO2CC6H4NMeSiMe3 added, and the cell charged with CO2 to approx. 760 psi. The cell was heated to 100°C and the pressure adjusted to 3,000 psi by further addition of CO2. The reaction yielded (p-MeO2CC6H4)2NMe in 84% yield after 17 h.

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

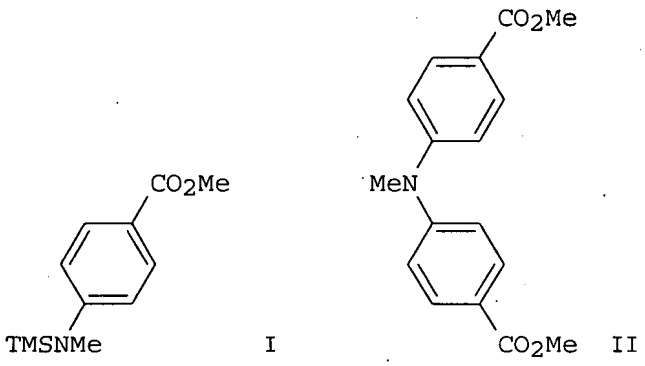
L9 ANSWER 4 OF 4 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 29



REF: Chemical Communications (Cambridge, United Kingdom), (17), 1976-1977; 2004
CON: 64 hours, 60 deg C

AN 141:366016 CASREACT
TI Palladium catalyzed cross-coupling reactions of silylamines
AU Smith, Catherine J.; Early, Tessa R.; Holmes, Andrew B.; Shute, Richard E.
CS Department of Chemistry, Melville Laboratory for Polymer Synthesis, Cambridge, CB2 1EW, UK
SO Chemical Communications (Cambridge, United Kingdom) (2004), (17), 1976-1977
CODEN: CHCOFS; ISSN: 1359-7345
PB Royal Society of Chemistry
DT Journal
LA English
GI



AB The palladium-catalyzed formation of C-N bonds to produce a range of aryl amines in supercrit. carbon dioxide is reported; carbamic acid formation is avoided in part by the use of N-silylamines as surrogates for the free amine. For example, the aromatic amination (coupling

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reaction) of 4-[methyl(trimethylsilyl)amino]benzoic acid Me ester (I) with 4-bromobenzoic acid Me ester gave 4,4'-(methylimino)bis[benzoic acid] Me ester (II).

RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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CAS ONLINE PRINTOUT

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(FILE 'HOME' ENTERED AT 07:36:41 ON 18 OCT 2007)

FILE 'CASREACT' ENTERED AT 07:37:09 ON 18 OCT 2007
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L2 17 S L1
L3 0 S FCRDREF
L4 628 S L1 FUL
L5 26908 S PALLADIUM
L6 68 S L5 AND L4

FILE 'REGISTRY' ENTERED AT 07:41:31 ON 18 OCT 2007
E CARBON DIOXIDE/CN
L7 1 S E3

FILE 'CASREACT' ENTERED AT 07:41:56 ON 18 OCT 2007
L8 5511 S L7
L9 4 S L8 AND L6

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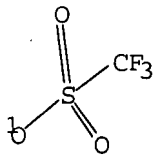
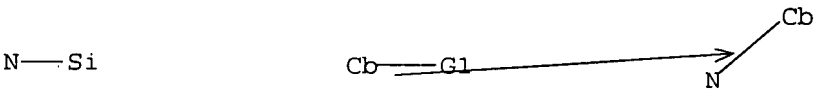
L1 HAS NO ANSWERS
L1 STR





G1 X,[@1]

Structure attributes must be viewed using STN Express query preparation.

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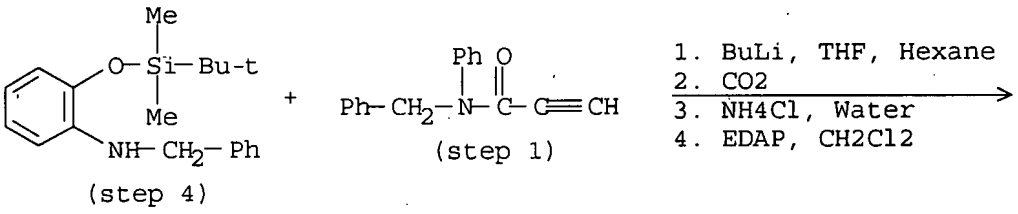
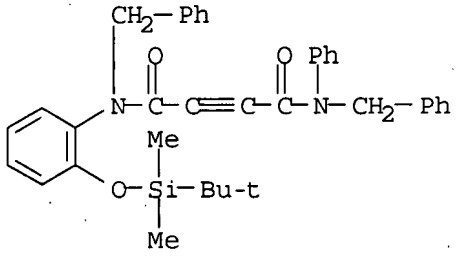
L9 ANSWER 1 OF 4 CASREACT COPYRIGHT 2007 ACS on STN

CAS ONLINE PRINTOUT

RX(25) OF 241

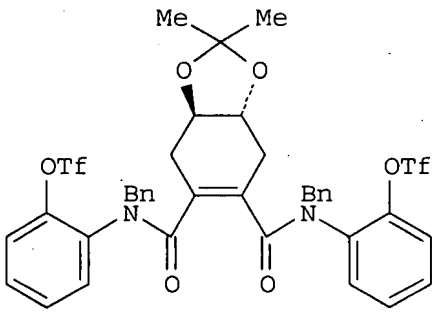




32%

REF: Journal of Organic Chemistry, 71(7), 2587-2599; 2006
CON: STAGE(1) 0.5 hours, -78 deg C
STAGE(2) 5 minutes, -78 deg C; -78 deg C -> room temperature
STAGE(4) -60 deg C; 2 hours, -60 deg C -> -5 deg C

GI



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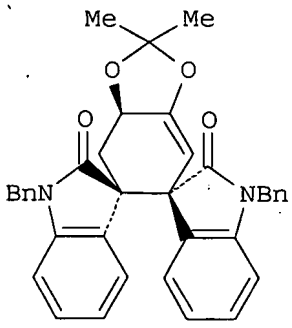


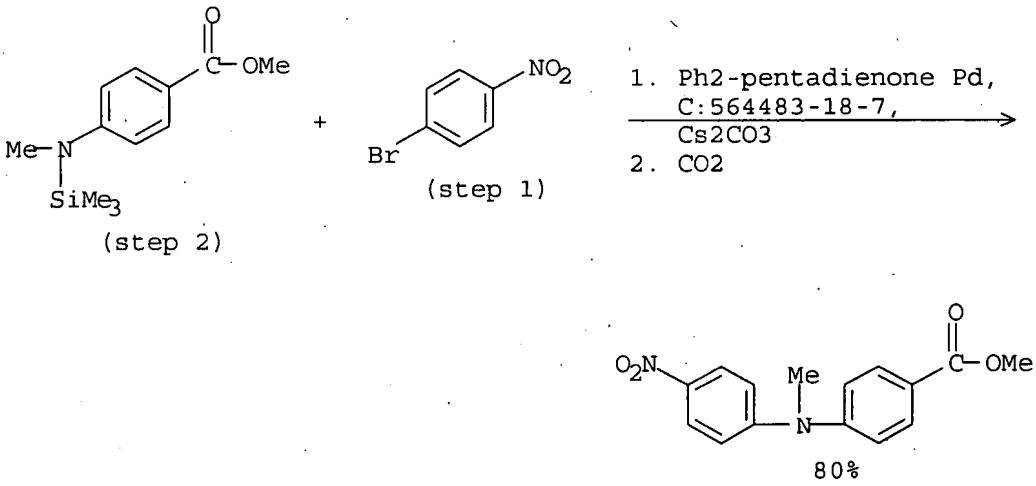
II

AB Diastereoselective double Heck cyclizations of cyclohexene diamides [e.g., trans-acetonide 1 (I) and its trans-disiloxy analog 3] form contiguous quaternary stereocenters (e.g., II from I), with diastereoselection being

controlled by the trans-diol protecting group. In this, the first in a series of two papers, the origin of diastereoselection in the first ring-closure step of these reactions is examined Nine simplified analogs of 1 and 3 were synthesized and cyclized to discern what structural features are required to realize high diastereoselection in the first intramol. Heck reaction. These studies show that high stereoselection (>20:1) does not arise from a single structural feature: it is seen only in substrates that contain both a trans-acetonide and a tertiary amide substituent at C2. Two subtle factors appear to be involved: avoidance of eclipsing interactions between the forming C-C bond and the pseudoaxial hydrogen atom at C6 and between the pseudoequatorial hydrogen atom at C6 and the carbonyl carbon of the forming spirooxindole. The vinylic amide substituent that is not involved in the insertion event preferentially adopts a perpendicular conformation, placing the sterically bulky NR2 over the alkene π bond. Syn-Pentane-like interactions between this substituent and the C3 of the cyclohexene are avoided in the favored insertion topog. These two effects, when combined, produce a highly diastereoselective process. Safety was recommend use of glass-lined steel reactor for preparation of diacid chloride intermediates for Heck cyclization substrates via Diels-Alder reaction.

L9 ANSWER 2 OF 4 CASREACT COPYRIGHT 2007 ACS on STN

RX(4) OF 73



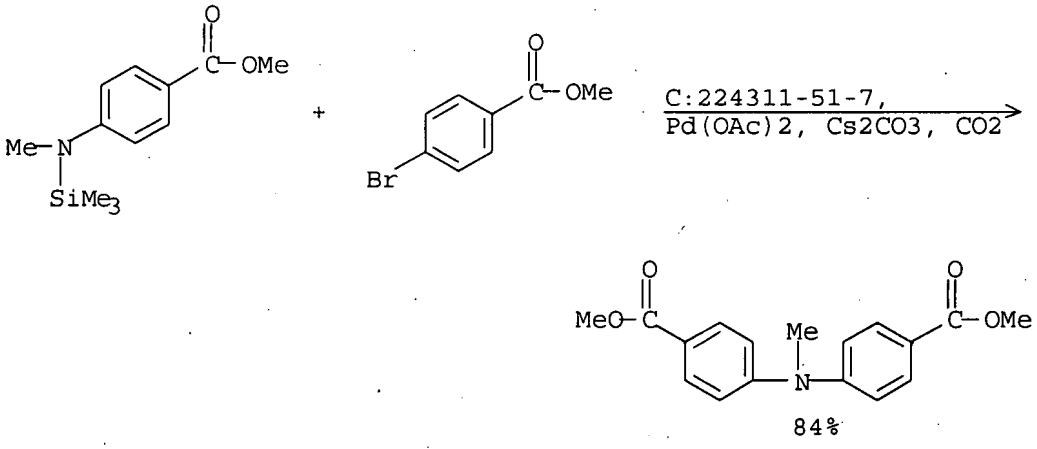
REF: Organic & Biomolecular Chemistry, 3(20), 3767-3781; 2005
NOTE: supercritical, green chemistry - solvent, high pressure in second stage, reaction in a sealed high pressure cell, incremental addition of solvent in second stage
CON: STAGE(1) room temperature
STAGE(2) 800 psi; 100 deg C, 800 psi; 800 psi -> 1800 psi; 17 hours, 100 deg C, 1800 psi; 100 deg C -> room temperature

AB Palladium catalyzed C-N bond formation in supercrit. carbon dioxide has been accomplished. Carbamic acid formation is avoided in part through the use of an N-silylamine as the coupling partner. Employing a catalyst system of Pd2dba3 (1 mol%) and 2-dicyclohexylphosphino-2',4',6'-triisopropyl-1,1'-biphenyl (X-Phos) (2 mol%) enabled the catalytic amination of aryl bromides and chlorides with N-silylanilines to be realized in excellent yield. Extension of the methodol. to the N-arylation of N-silyldiarylamines, N-silylazoles and N-silylsulfonamides is reported.

L9 ANSWER 3 OF 4 CASREACT COPYRIGHT 2007 ACS on STN

CAS ONLINE PRINTOUT

RX(1) OF 24

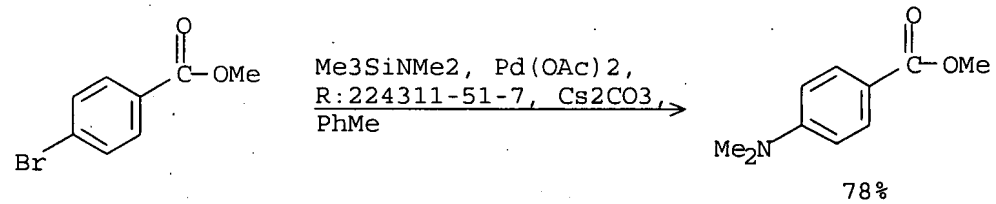


REF: PCT Int. Appl., 2005090283, 29 Sep 2005
NOTE: high pressure, yield depends on reaction pressure, supercritical CO2 used as solvent
CON: 17 hours, 100 deg C, 3000 psi

AB A method for synthesizing amines R1NR2R3 (R1 is optionally substituted aryl; R2 is optionally substituted aryl, heterocyclyl, alkyl or sulfonyl; R3 is H or optionally substituted alkyl, heterocyclyl or aryl; or R2R3N is optionally substituted heterocyclyl or heteroaryl) comprises reacting R1-L, where L is a labile leaving group, with a silylamine R2R3NSiR4R5R6 (R4, R5, R6 are independently optionally substituted alkyl, aryl, heterocyclyl, hydroxy, halo, amino or alkoxy or two of R1, R2 and R3, together with the silicon atom may form a ring) in compressed carbon dioxide in the presence of a transition metal catalyst and a base. Thus, a stainless steel cell containing Me p-bromobenzoate, Cs2CO3, palladium acetate, and di-tert-butylbiphenylphosphine was evacuated and refilled with nitrogen, p-MeO2CC6H4NMeSiMe3 added, and the cell charged with CO2 to approx. 760 psi. The cell was heated to 100°C and the pressure adjusted to 3,000 psi by further addition of CO2. The reaction yielded (p-MeO2CC6H4)2NMe in 84% yield after 17 h.

L9 ANSWER 4 OF 4 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 29



REF: Chemical Communications (Cambridge, United Kingdom), (17), 1976-1977; 2004
CON: 64 hours, 60 deg C

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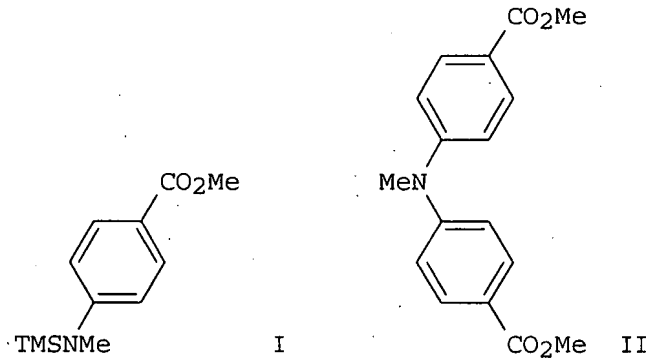

AB The palladium-catalyzed formation of C-N bonds to produce a range of aryl amines in supercrit. carbon dioxide is reported; carbamic acid formation is avoided in part by the use of N-silylamines as surrogates for the free amine. For example, the aromatic amination (coupling reaction) of 4-[methyl(trimethylsilyl)amino]benzoic acid Me ester (I) with 4-bromobenzoic acid Me ester gave 4,4'-(methylimino)bis[benzoic acid] Me ester (II).

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CAS ONLINE PRINTOUT

=> d his

(FILE 'HOME' ENTERED AT 07:36:41 ON 18 OCT 2007)

FILE 'CASREACT' ENTERED AT 07:37:09 ON 18 OCT 2007

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L6	68	S L5 AND L4

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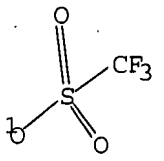

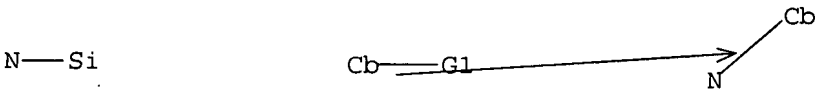

G1 X,[@1]

Structure attributes must be viewed using STN Express query preparation.

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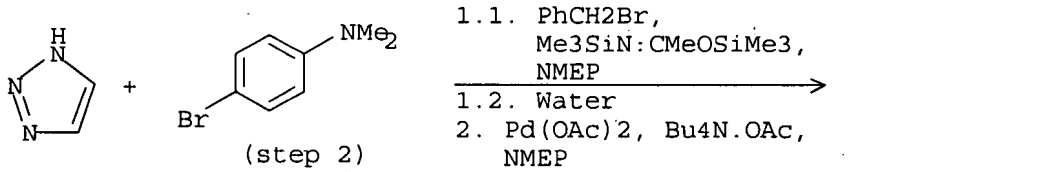
L6 ANSWER 1 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(25) OF 28 - 2 STEPS



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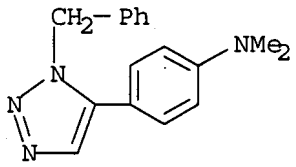


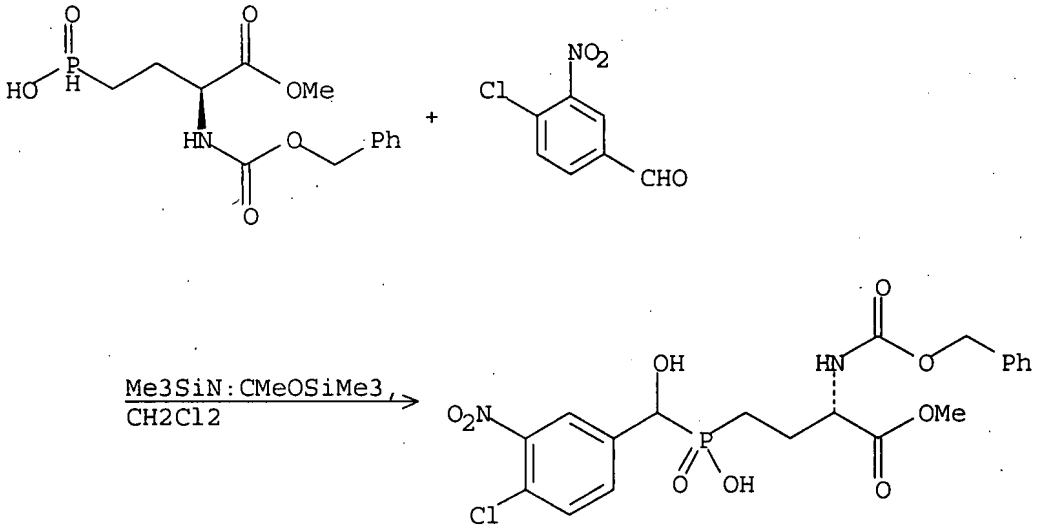
83%

REF: Organic Letters, 9(12), 2333-2336; 2007
CON: STEP(1) overnight, 100 deg C
STEP(2) 100 deg C

CAS ONLINE PRINTOUT

L6 ANSWER 2 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

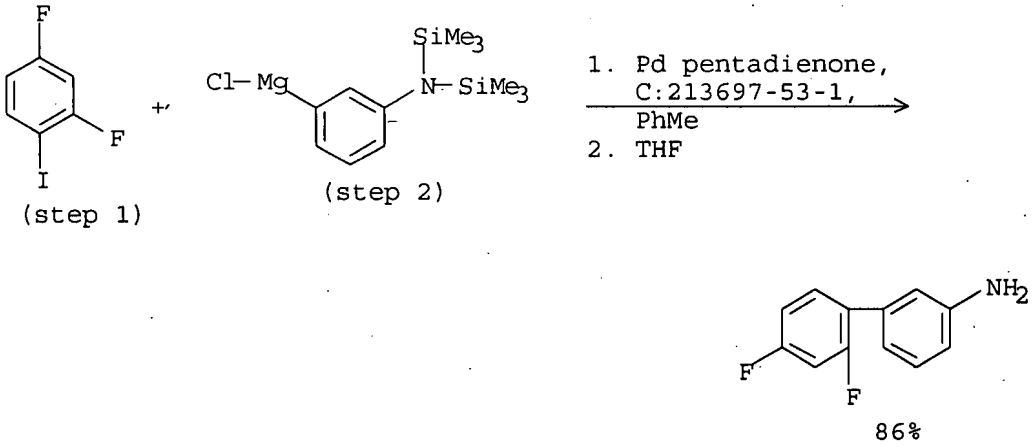
RX(41) OF 244



REF: PCT Int. Appl., 2007052169, 10 May 2007
CON: STAGE(1) 0 deg C; 0 deg C -> room temperature; overnight, room temperature

L6 ANSWER 3 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(10) OF 23

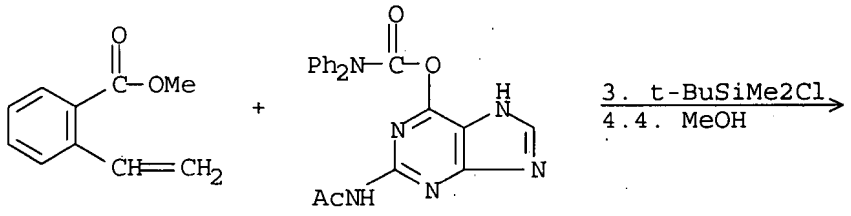


REF: Journal of the American Chemical Society, 129(13), 3844-3845; 2007
NOTE: Kumada-Corriu Cross-Coupling reaction
CON: STAGE(1) 20 minutes, 60 deg C; 60 deg C -> -20 deg C
STAGE(2) 14 hours, -20 deg C; -20 deg C -> room temperature

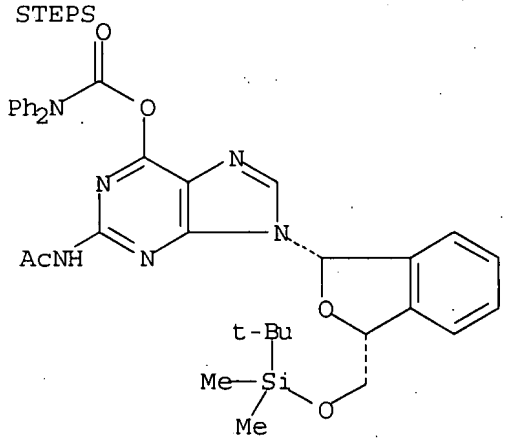
L6 ANSWER 4 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

CAS ONLINE PRINTOUT

RX(68) OF 91 - 5 STEPS



RX(68) OF 91 - 5 STEPS



stereoisomers

20%

REF: Chinese Journal of Chemistry, 24(4), 504-508; 2006

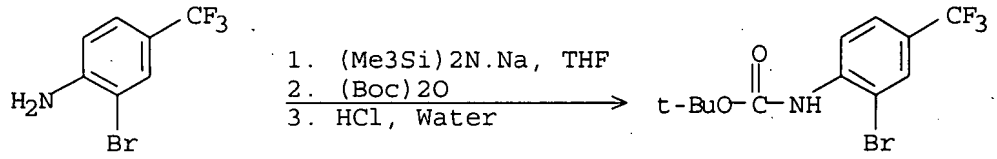
NOTE: 2) alternate reaction with lower yield shown, 4) 78% overall yield in five steps from methyl-2-iodobezoate, Dowex 50W (H+) form used in stage 4, 5) stereoselective, regioselective

CON: STEP(1) 12 hours, room temperature
STEP(2.1) 1 hour, room temperature
STEP(2.2) neutralized
STEP(3) 6 hours, room temperature
STEP(4.1) -45 deg C; 1 hour, -45 deg C
STEP(4.2) 0.5 hours, room temperature
STEP(4.3) 1 hour, room temperature
STEP(4.4) 1 hour, room temperature
STEP(5.1) 0.5 hours, 80 deg C
STEP(5.2) 0 deg C; 1 hour, room temperature

L6 ANSWER 5 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

CAS ONLINE PRINTOUT

RX(7) OF 61

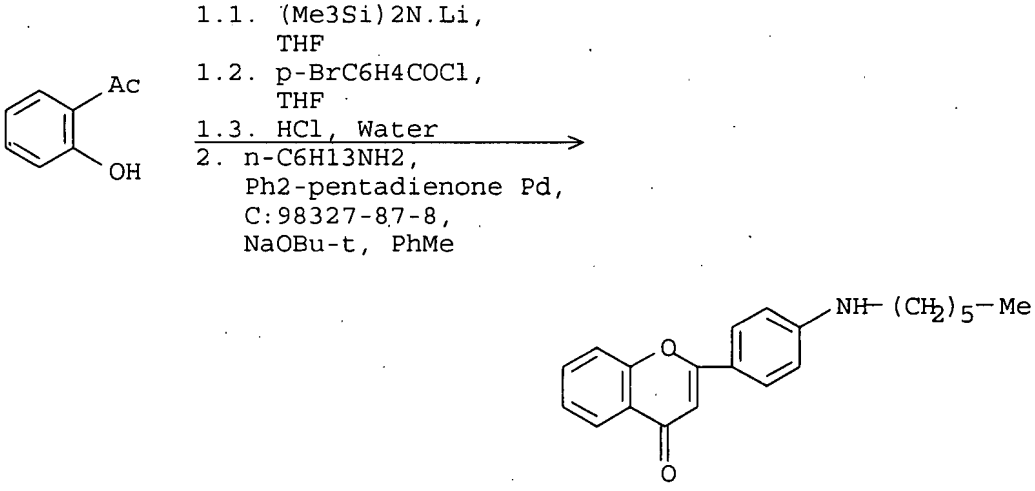


(step 1) 96%

REF: Synthesis, (22), 3895-3901; 2006
CON: STAGE(1) 15 minutes, room temperature
STAGE(2) overnight, room temperature

L6 ANSWER 6 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(33) OF 55 - 2 STEPS



84%

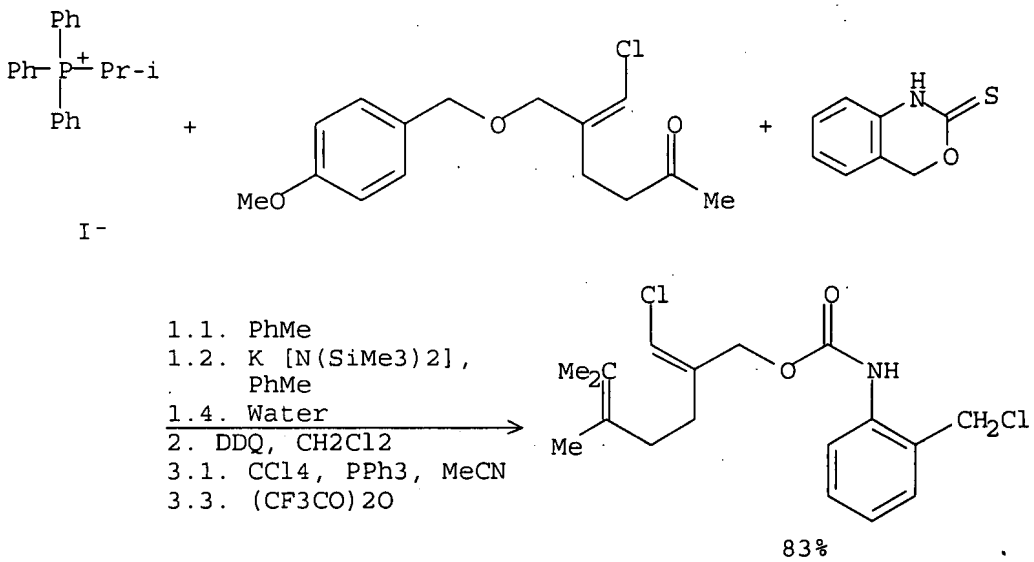
REF: Chemical Communications (Cambridge, United Kingdom), (46), 4814-4816; 2006

NOTE: 2) Buchwald-Hartwig amination, microwave irradiation
CON: STEP(1.1) 0.5 hours, -78 deg C; 2 hours, -20 deg C; -20 deg C -> -78 deg C
STEP(1.2) 1 hour, -78 deg C; 2 hours, room temperature
STEP(1.3) cooled
STEP(2) 15 minutes, 110 deg C

L6 ANSWER 7 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

CAS ONLINE PRINTOUT

RX(36) OF 81 - 3 STEPS



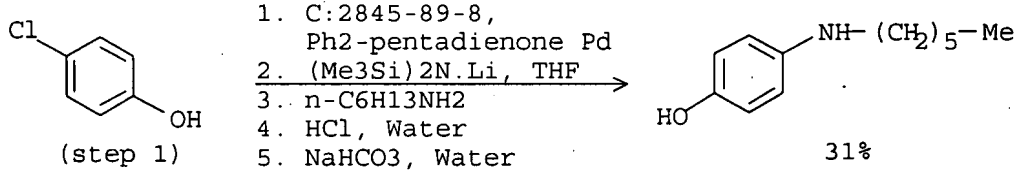
83%

REF: European Journal of Organic Chemistry, (21), 4916-4923; 2006

NOTE: 2) pH=7 buffer used in first stage
CON: STEP(1.1) room temperature -> 0 deg C
STEP(1.2) 30 minutes, 0 deg C
STEP(1.3) 16 hours, room temperature
STEP(2) 60 minutes, room temperature, pH 7
STEP(3.1) 3 hours, 50 deg C; 50 deg C -> 0 deg C
STEP(3.2) 40 hours, 50 deg C; cooled
STEP(3.3) 4 hours, room temperature

L6 ANSWER 8 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 33



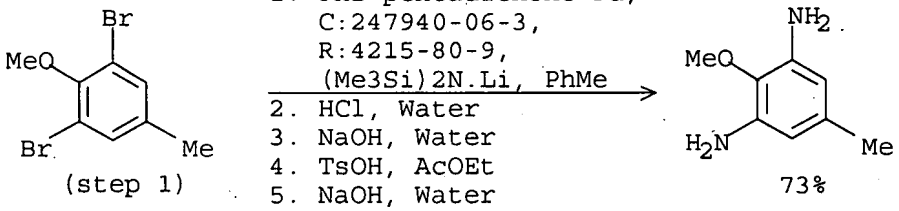
31%

REF: Angewandte Chemie, International Edition, 45(39), 6523-6527; 2006
NOTE: chemoselective
CON: STAGE(1) room temperature
STAGE(2) 5 minutes, room temperature
STAGE(3) 24 hours, 40 deg C; 40 deg C -> room temperature
STAGE(4) 5 minutes, room temperature
STAGE(5) room temperature, pH 7

L6 ANSWER 9 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

CAS ONLINE PRINTOUT

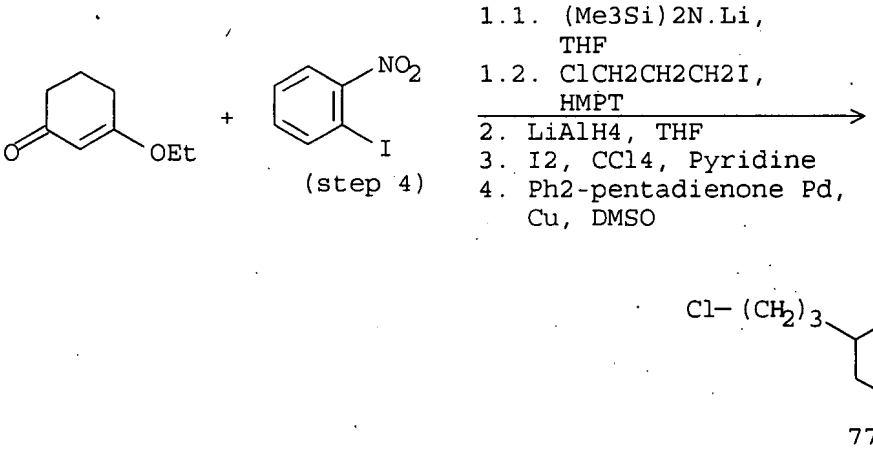
RX(1) OF 9



REF: U.S. Pat. Appl. Publ., 2006258888, 16 Nov 2006
CON: STAGE(1) 17 hours, room temperature -> 100 deg C;
100 deg C -> 25 deg C
STAGE(2) 5 minutes, room temperature
STAGE(3) 5 minutes, room temperature, pH 12
STAGE(4) room temperature
STAGE(5) room temperature, pH 12

L6 ANSWER 10 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(143) OF 450 - 4 STEPS

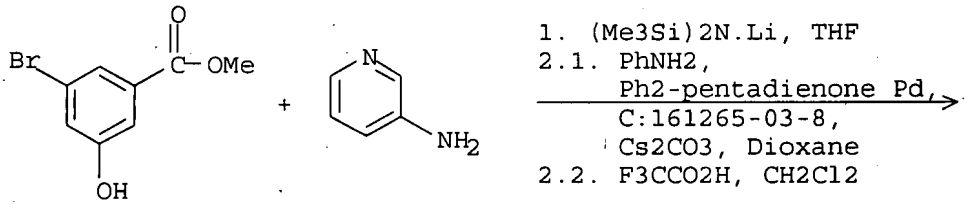


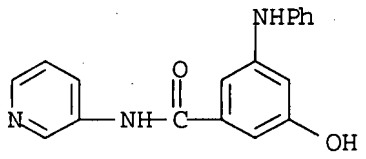
REF: Australian Journal of Chemistry, 58(10), 722-737; 2005
NOTE: 1) regioselective, 2) exothermic, 3) regioselective, 4) Ullmann cross-coupling reaction
CON: STEP(1.1) room temperature -> -30 deg C; 0.5 hours, -30 deg C
STEP(1.2) -30 deg C; 16 hours, -30 deg C -> 18 deg C
STEP(2.1) 0 deg C; 0.5 hours, 18 deg C
STEP(3.1) 18 deg C; 16 hours, 18 deg C
STEP(4.1) 2 hours, 70 deg C; 70 deg C -> 18 deg C

L6 ANSWER 11 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

CAS ONLINE PRINTOUT

RX(39) OF 61 - 2 STEPS



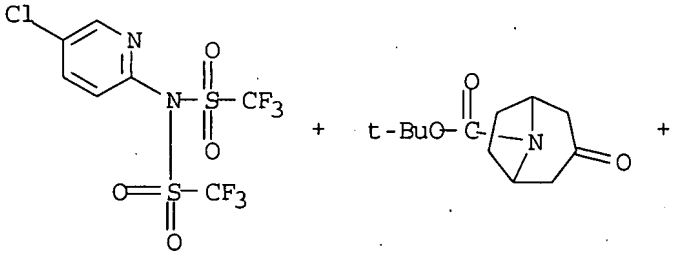


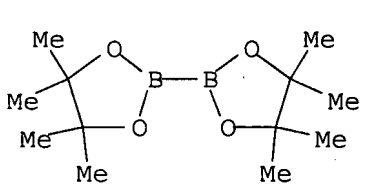
24%

REF: Tetrahedron Letters, 47(28), 4897-4901; 2006
NOTE: 1) combinatorial, solid-supported reaction, 2) combinatorial, solid-supported reaction
CON: STEP(1) 3 hours, 60 deg C
STEP(2.1) 16 hours, 60 deg C
STEP(2.2) 3 minutes, room temperature

L6 ANSWER 12 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

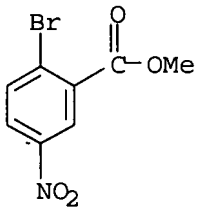
RX(40) OF 52 - 3 STEPS





(step 2)

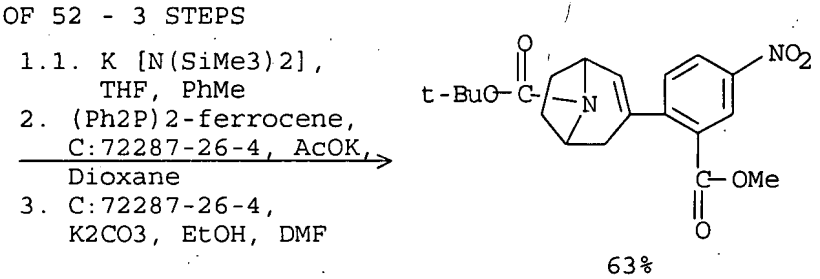
+



(step 3)

CAS ONLINE PRINTOUT

RX(40) OF 52 - 3 STEPS

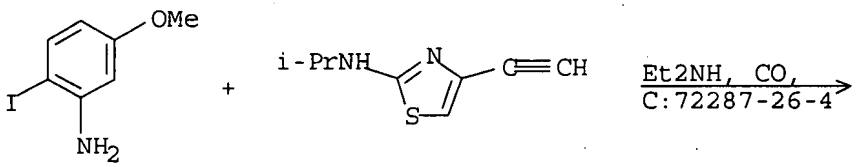


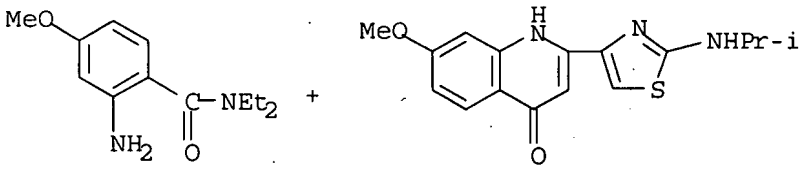
63%

REF: Canadian Journal of Chemistry, 84(4), 555-560; 2006
NOTE: 3) Suzuki-Miyaura coupling reaction
CON: STEP(1.1) 30 minutes, -78 deg C; 3.5 hours, -78 deg C
STEP(1.2) 4 hours, -78 deg C; overnight,
-78 deg C -> room temperature
STEP(2.1) 20 minutes, room temperature; 8 - 10 hours, 80 deg C
STEP(3.1) 5 - 10 minutes, room temperature; 3 - 16 hours,
100 deg C

L6 ANSWER 13 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(8) OF 30



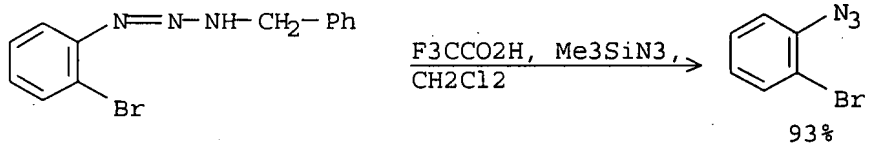


3% 73%

REF: Journal of Organic Chemistry, 71(13), 5031-5034; 2006
NOTE: high pressure, optimization study, optimized on palladium
catalyst and reaction conditions
CON: 6 hours, 120 deg C, 250 psi

L6 ANSWER 14 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(7) OF 148



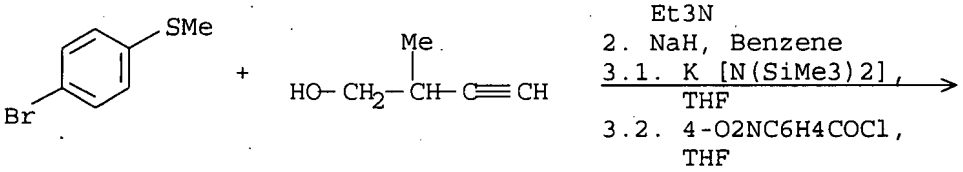
93%

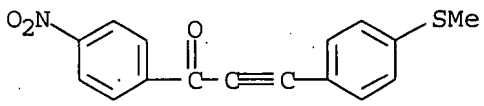
REF: European Journal of Organic Chemistry, (8), 1886-1898; 2006
NOTE: solid-supported reactant
CON: 30 minutes, room temperature

CAS ONLINE PRINTOUT

L6 ANSWER 15 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(140) OF 260 - 3 STEPS



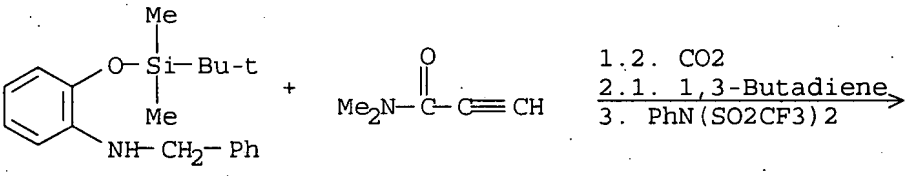


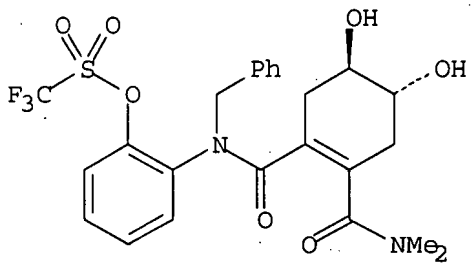
21%

REF: Journal of Medicinal Chemistry, 49(5), 1668-1683; 2006
CON: STEP(1.1) 25 deg C; 6 hours, 70 - 75 deg C
STEP(2) 1 hour, 105 - 110 deg C
STEP(3.1) -78 deg C; 3 minutes, -78 deg C
STEP(3.2) -78 deg C; -78 deg C -> room temperature; overnight, room temperature

L6 ANSWER 16 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(157) OF 241 - 4 STEPS





78%

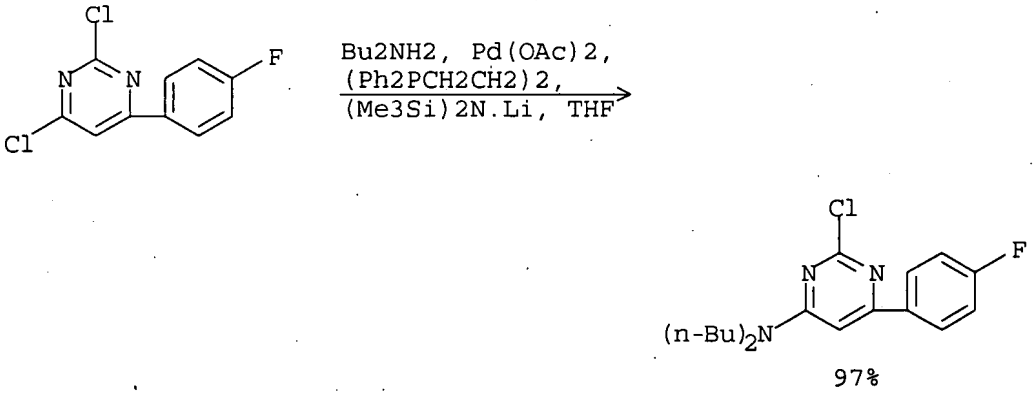
REF: Journal of Organic Chemistry, 71(7), 2587-2599; 2006

CAS ONLINE PRINTOUT

NOTE: 2) safety, Diels-Alder reaction, 4) stereoselective
CON: STEP(1.1) 0.5 hours, -78 deg C
STEP(1.2) 5 minutes, -78 deg C; -78 deg C -> room temperature
STEP(1.4) 1 hour, -60 deg C -> -5 deg C
STEP(2.1) -78 deg C; -78 deg C -> room temperature; 48 hours, room temperature
STEP(3) 1 hour, room temperature
STEP(4.1) 20 minutes, 0 deg C; 4 hours, room temperature
STEP(4.3) 12 hours, 80 deg C

L6 ANSWER 17 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(2) OF 52

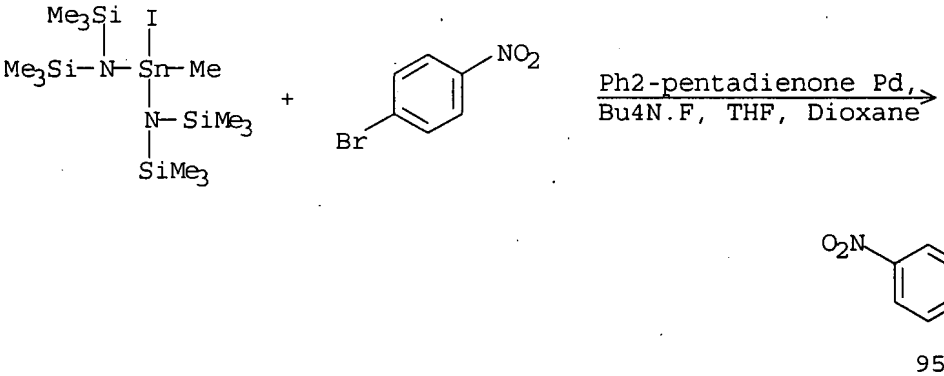


97%

REF: Organic Letters, 8(3), 395-398; 2006
NOTE: regioselective, optimization study, optimized on palladium catalyst, ligand, and catalyst loading
CON: 5 minutes, 0 deg C

L6 ANSWER 18 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(4) OF 24



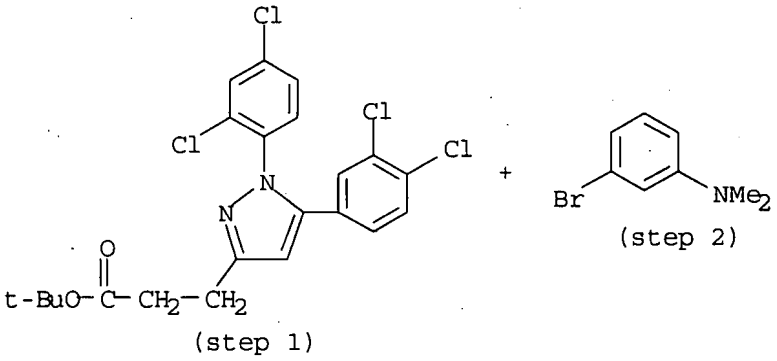
95%

REF: Chemical Communications (Cambridge, United Kingdom), (1), 97-99; 2006
CON: 30 minutes, reflux

CAS ONLINE PRINTOUT

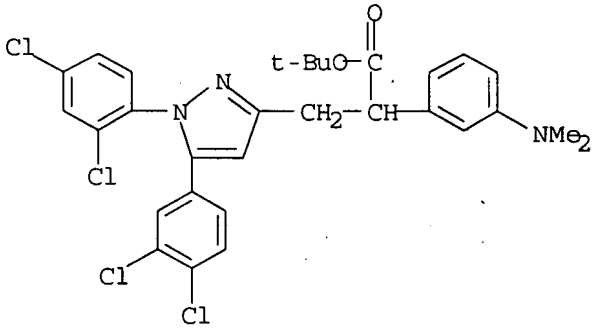
L6 ANSWER 19 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(55) OF 255



1. C:213697-53-1, Pd(OAc)2, (Me3Si)2N.Li, THF, PhMe
2. PhMe
3. NH4Cl, Water

RX(55) OF 255



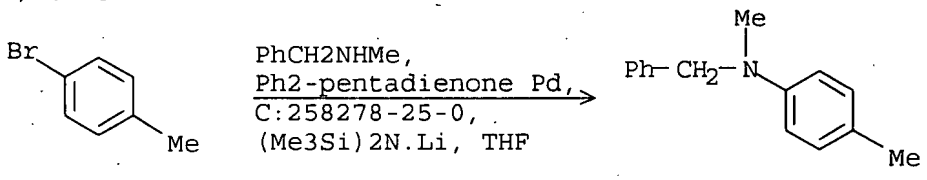
16%

REF: U.S. Pat. Appl. Publ., 2006004195, 05 Jan 2006
CON: STAGE(1) -10 deg C; 0.17 hours, -10 deg C
STAGE(2) room temperature; 3 hours, room temperature -> 80 deg C

L6 ANSWER 20 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

CAS ONLINE PRINTOUT

RX(4) OF 37

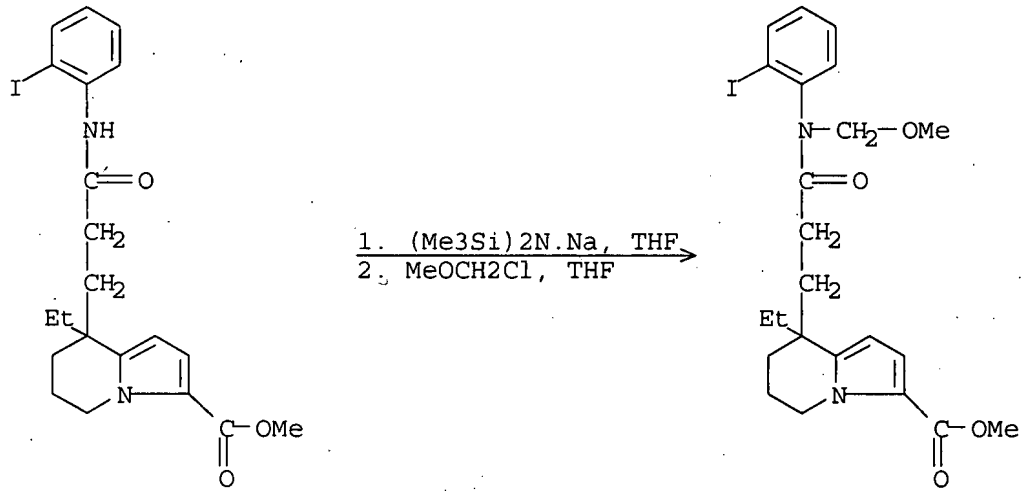


73%

REF: Journal of Organometallic Chemistry, 690(24-25), 5841-5848; 2005
CON: 24 hours, 22 deg C

L6 ANSWER 21 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(5) OF 28



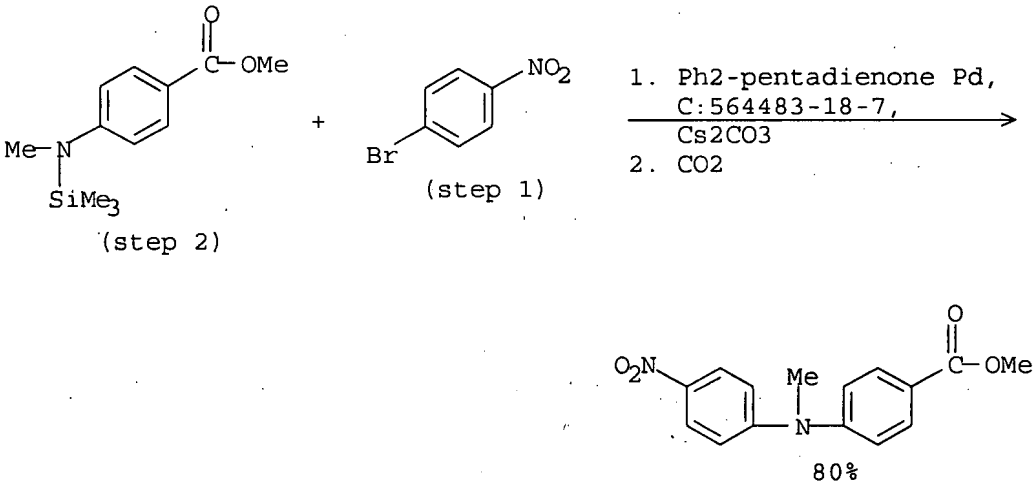
(step 1) 85%

REF: Organic Letters, 7(23), 5207-5209; 2005
NOTE: key intermediate
CON: STAGE(1) 30 minutes, 0 deg C
STAGE(2) 10 minutes, 0 deg C; 1 hour, 0 deg C -> room temperature

L6 ANSWER 22 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

CAS ONLINE PRINTOUT

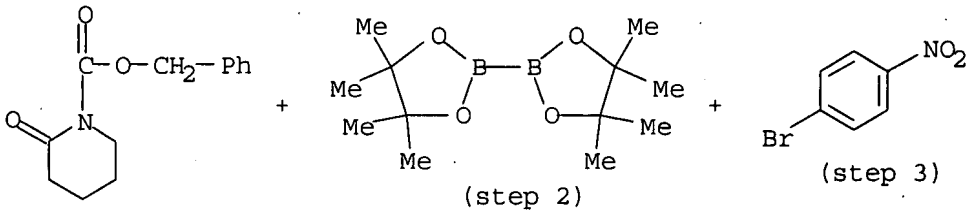
RX(4) OF 73

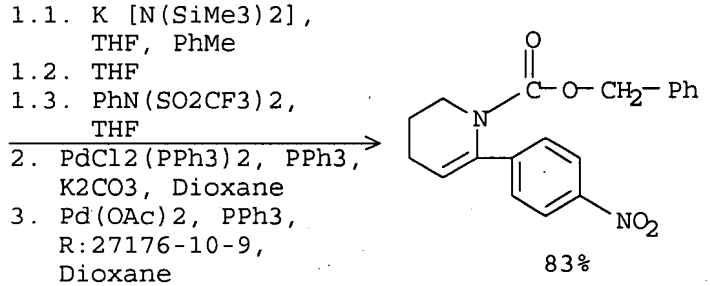


REF: Organic & Biomolecular Chemistry, 3(20), 3767-3781; 2005
NOTE: supercritical, green chemistry - solvent, high pressure in second stage, reaction in a sealed high pressure cell, incremental addition of solvent in second stage
CON: STAGE(1) room temperature
STAGE(2) 800 psi; 100 deg C, 800 psi; 800 psi -> 1800 psi; 17 hours, 100 deg C, 1800 psi; 100 deg C -> room temperature

L6 ANSWER 23 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(117) OF 176 - 3 STEPS





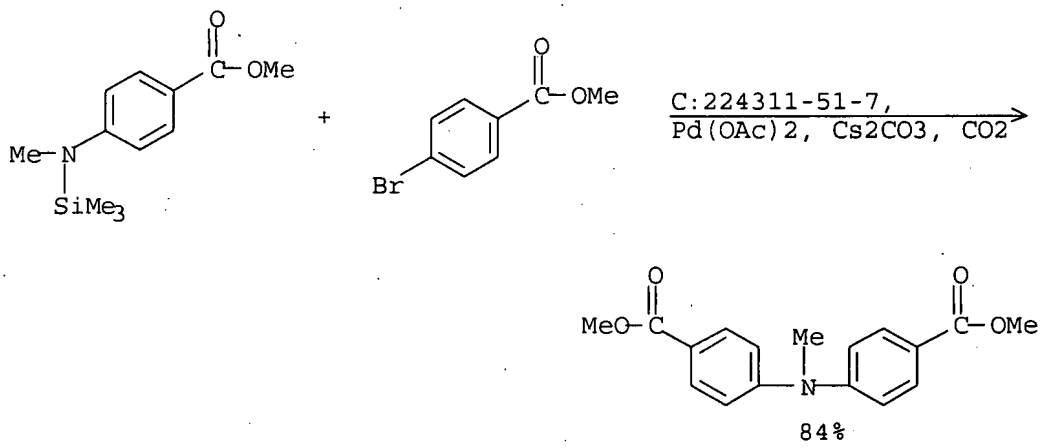
REF: Journal of Organic Chemistry, 70(18), 7324-7330; 2005

NOTE: 2) optimization study(optimized on reagent, solvent, temperature), alternate preparations also described
CON: STEP(1.1) room temperature -> -78 deg C
STEP(1.2) 1.5 hours, -78 deg C
STEP(1.3) -78 deg C; 1 hour, -78 deg C; 1 hour, -78 deg C -> room temperature
STEP(2) 7 hours, room temperature -> 90 deg C
STEP(3) 1.5 hours, 100 deg C

CAS ONLINE PRINTOUT

L6 ANSWER 24 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

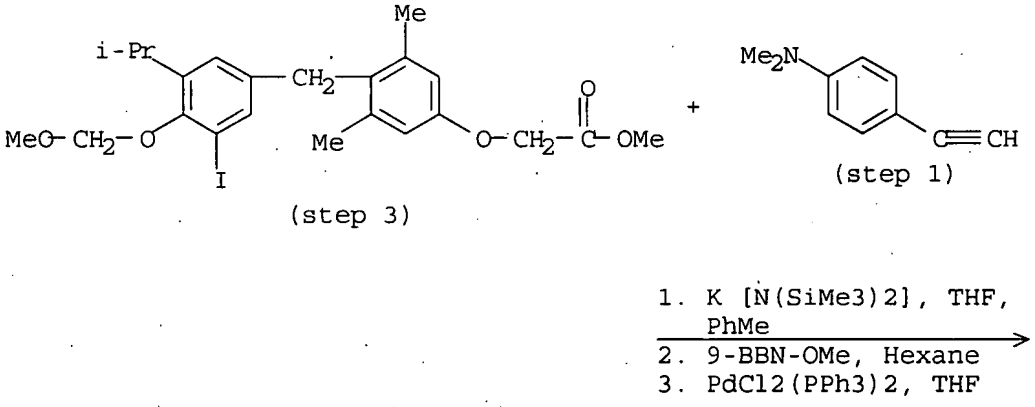
RX(1) OF 24



REF: PCT Int. Appl., 2005090283, 29 Sep 2005
NOTE: high pressure, yield depends on reaction pressure, supercritical CO2 used as solvent
CON: 17 hours, 100 deg C, 3000 psi

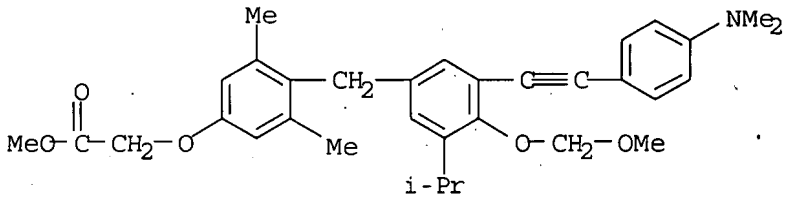
L6 ANSWER 25 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(27) OF 633



CAS ONLINE PRINTOUT

RX(27) OF 633

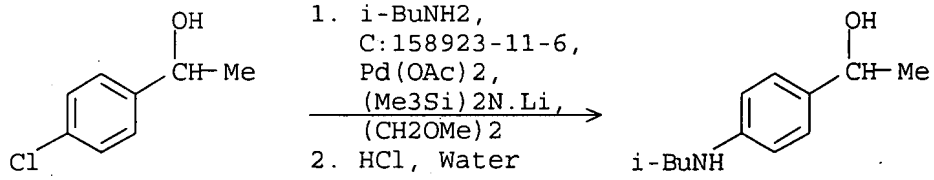


76%

REF: Journal of the American Chemical Society, 127(13), 4599-4608; 2005
NOTE: Suzuki-Miyaura reaction third stage
CON: STAGE(1) 30 minutes, -78 deg C
STAGE(2) 2 hours, -78 deg C
STAGE(3) 24 hours, reflux

L6 ANSWER 26 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(50) OF 67

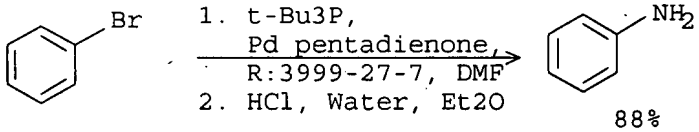


(step 1) 90%

REF: Angewandte Chemie, International Edition, 44(9), 1371-1375, S1371/1-S1371/79; 2005
CON: STAGE(1) 18 hours, 100 deg C; 100 deg C -> room temperature
STAGE(2) 5 minutes, room temperature
STAGE(3) room temperature, neutralized

L6 ANSWER 27 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 60



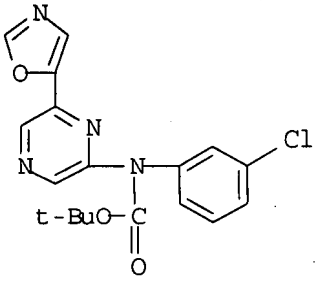
88%

REF: Organic Letters, 7(6), 1169-1172; 2005
CON: STAGE(1) 30 hours, 50 deg C
STAGE(2) neutralized

L6 ANSWER 28 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

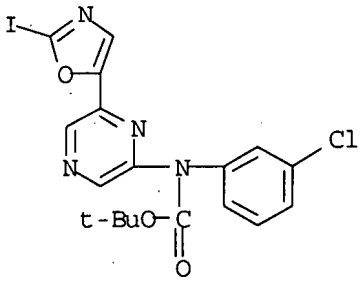
CAS ONLINE PRINTOUT

RX(60) OF 277



(step 1)

1. (Me3Si)2N.Li, THF
2. ICH2CH2I, THF
3. Na2S2O3

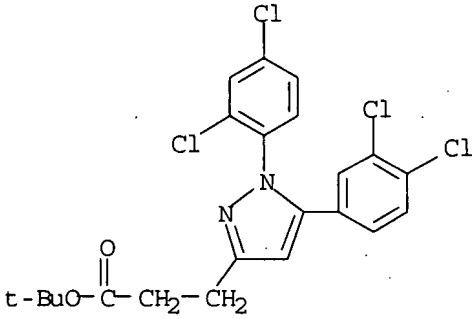


68%

REF: Journal of Medicinal Chemistry, 48(6), 1886-1900; 2005
CON: STAGE(1) -78 deg C; 1 hour, -78 deg C
STAGE(2) 1 hour, -78 deg C

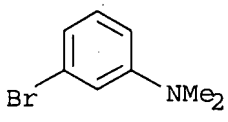
L6 ANSWER 29 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(107) OF 573



(step 2)

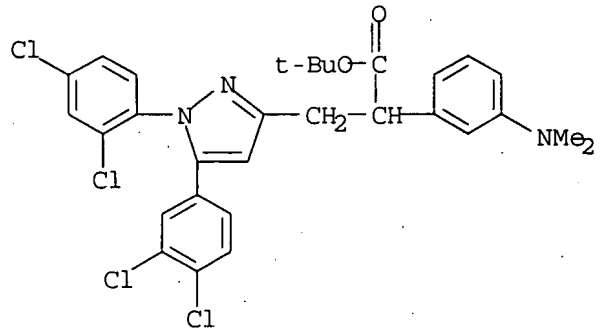
+



(step 3)

1. Pd(OAc)2, R:213697-53-1, (Me3Si)2N.Li, THF, PhMe
2. PhMe
3. PhMe
4. NH4Cl, Water

RX(107) OF 573

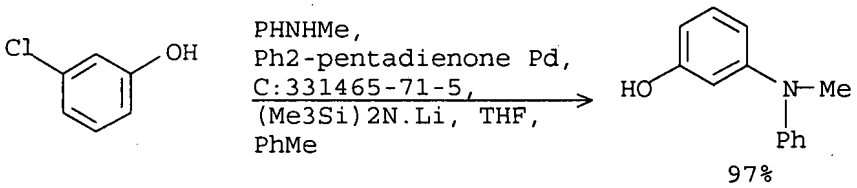


16%

REF: PCT Int. Appl., 2005005393, 20 Jan 2005
CON: STAGE(1) -10 deg C
STAGE(2) 10 minutes, -10 deg C
STAGE(3) -10 deg C -> room temperature;
room temperature -> 80 deg C; 3 hours, 80 deg C;
80 deg C -> room temperature
STAGE(4) room temperature

L6 ANSWER 30 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(2) OF 20



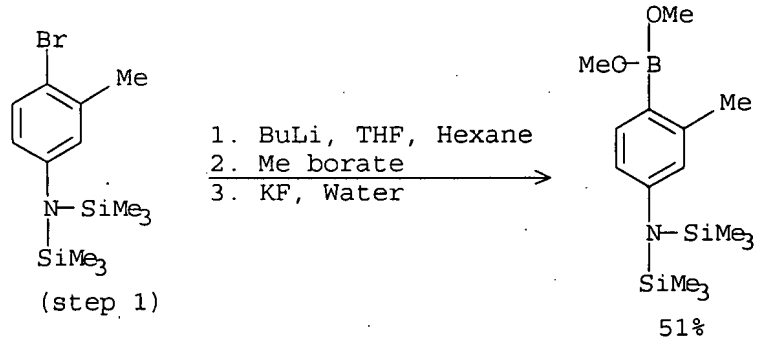
97%

REF: Advanced Synthesis & Catalysis, 346(6), 611-616; 2004
CON: 29 hours, 100 deg C

L6 ANSWER 31 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

CAS ONLINE PRINTOUT

RX(8) OF 14



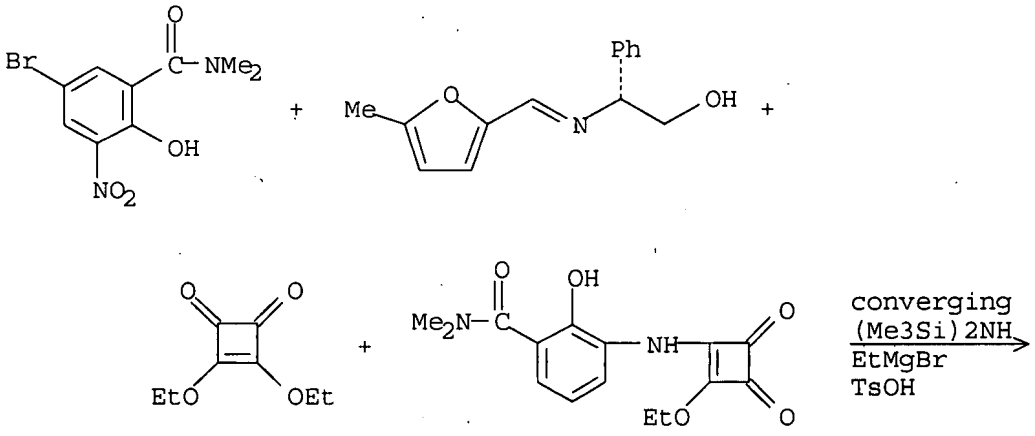
(step 1)

51%

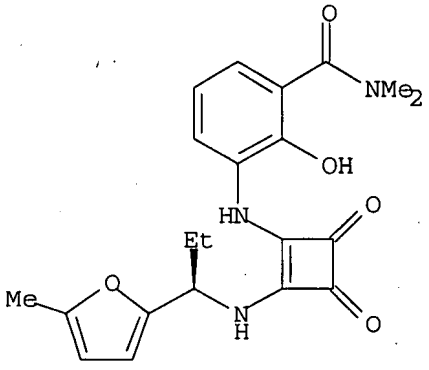
REF: Eur. Pat. Appl., 1479686, 24 Nov 2004
CON: STAGE(1) 10 minutes, -78 deg C -> -50 deg C
STAGE(2) 1 hour, -50 deg C
STAGE(3) room temperature

L6 ANSWER 32 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(46) OF 52 - 7 STEPS



RX(46) OF 52 - 7 STEPS



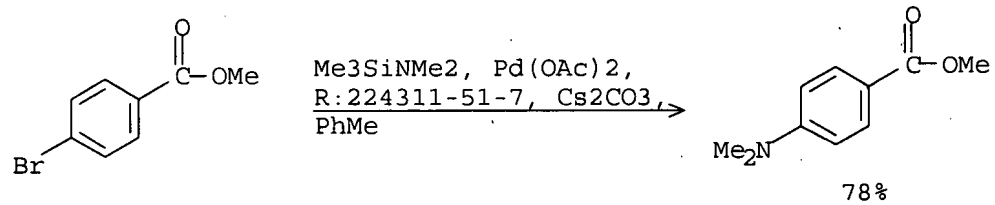
82%

REF: U.S. Pat. Appl. Publ., 2004209946, 21 Oct 2004

NOTE: workup, workup
CON: STEP(1.1) room temperature; 0.5 hours, room temperature; 2 hours, reflux
STEP(2) <35 deg C
STEP(3) 1 hour
STEP(4.1) room temperature -> 0 deg C; 2 hours, room temperature
STEP(5.1) 1 - 4 hour, 25 deg C
STEP(5.2) 6 - 14 hours, 25 deg C
STEP(6.1) 20 minutes, <30 deg C
STEP(6.2) 12 hours, 65 deg C
STEP(7.1) 10 hours, room temperature, 105 psi; room temperature -> 5 deg C
STEP(7.2) 2 hours, 25 deg C

L6 ANSWER 33 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 29

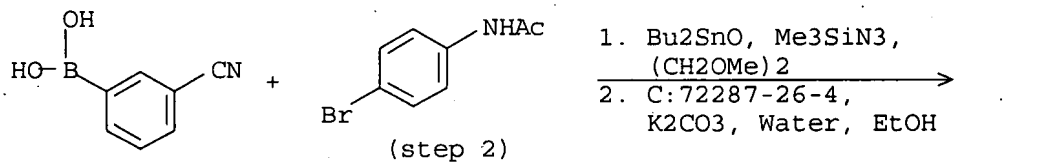


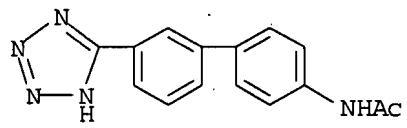
78%

REF: Chemical Communications (Cambridge, United Kingdom), (17), 1976-1977; 2004
CON: 64 hours, 60 deg C

L6 ANSWER 34 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(23) OF 23 - 2 STEPS





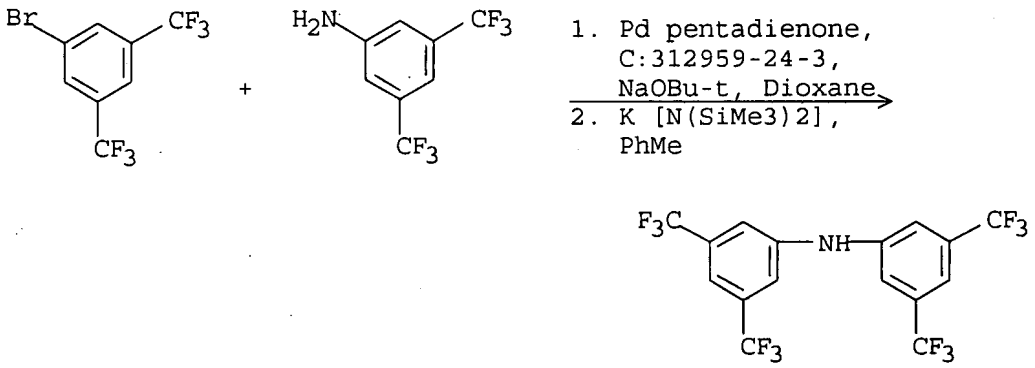
74%

REF: Organic Letters, 6(19), 3265-3268; 2004
NOTE: 1) microwave irradiation, optimization study, 2) Suzuki coupling, microwave irradiation
CON: STEP(1) 10 minutes, 150 deg C
STEP(2) 6 minutes, 150 deg C

L6 ANSWER 35 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

CAS ONLINE PRINTOUT

RX(29) OF 55 - 2 STEPS



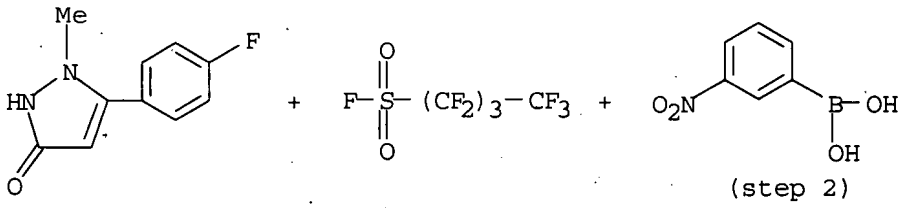
K

93%

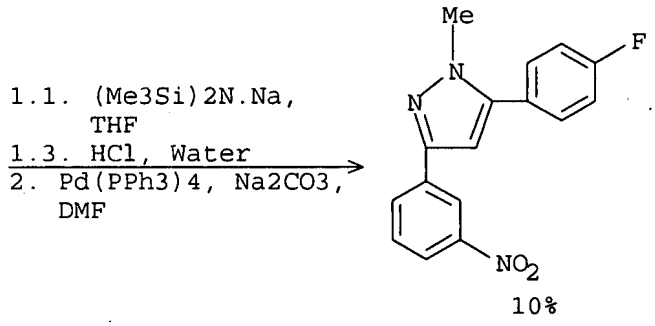
REF: Journal of the American Chemical Society, 126(17), 5344-5345; 2004
CON: STEP(1) 21.5 hours, 80 deg C
STEP(2) 3 hours, room temperature

L6 . ANSWER 36 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(38) OF 100 - 2 STEPS



(step 2)



10%

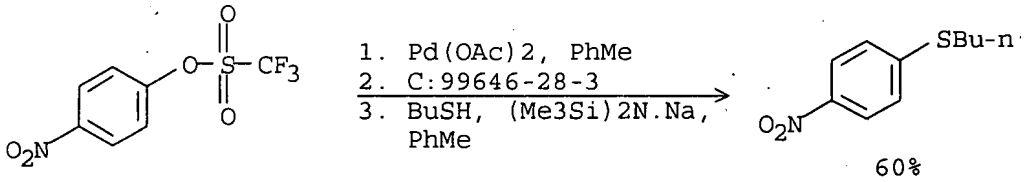
REF: Synlett, (5), 795-798; 2004

NOTE: 2) Suzuki reaction
CON: STEP(1.1) 5 minutes, 0 deg C
STEP(1.2) 2 - 4 hours, 0 deg C -> room temperature
STEP(1.3) room temperature
STEP(2) 18 hours, 100 deg C

CAS ONLINE PRINTOUT

L6 ANSWER 37 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(8) OF 12

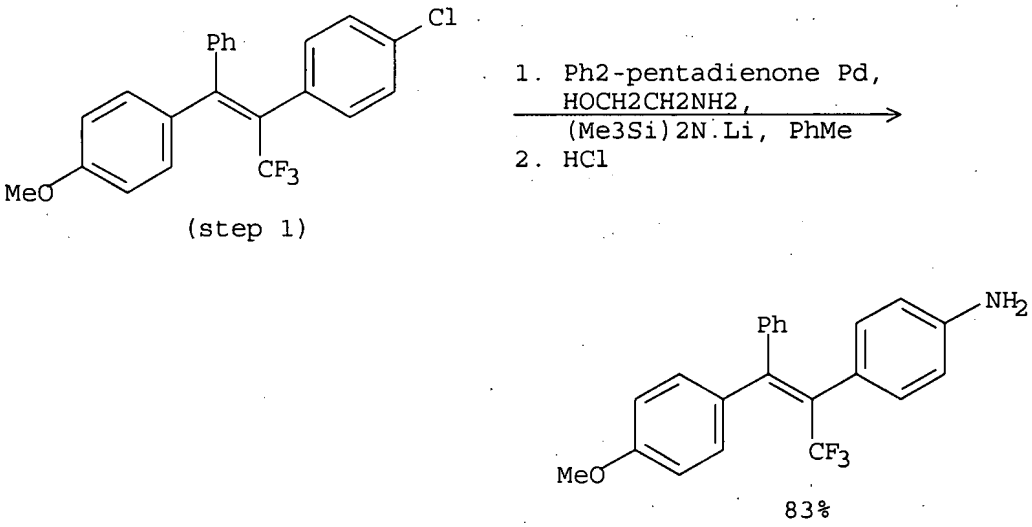


(step 1)

REF: Organic Syntheses, 2002, 79,, 43-51; 2003
CON: STAGE(1) 15 minutes, room temperature
STAGE(2) 15 minutes, room temperature
STAGE(3) 3 minutes, 21 deg C; 21 deg C -> 28 deg C;
28 deg C -> 100 deg C; 12 hours, 100 deg C;
100 deg C -> room temperature

L6 ANSWER 38 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(24) OF 51



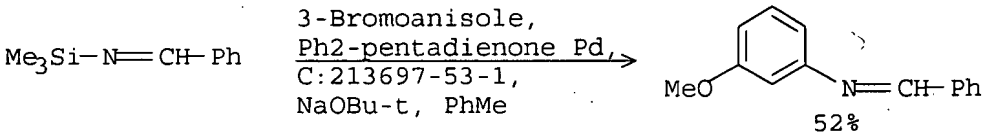
(step 1)

REF: Angewandte Chemie, International Edition, 43(7), 879-882; 2004
CON: 12 hours, 100 deg C

L6 ANSWER 39 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

CAS ONLINE PRINTOUT

RX(1) OF 15

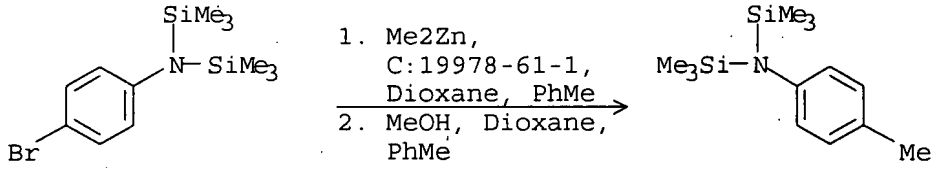


52%

REF: Angewandte Chemie, International Edition, 43(3), 343-345; 2004
NOTE: alternative reaction conditions shown, optimization study, optimized on ligand
CON: 14 hours, 90 deg C

L6 ANSWER 40 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(11) OF 23

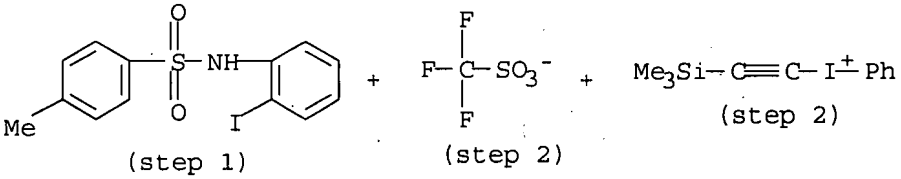


(step 1) 81%

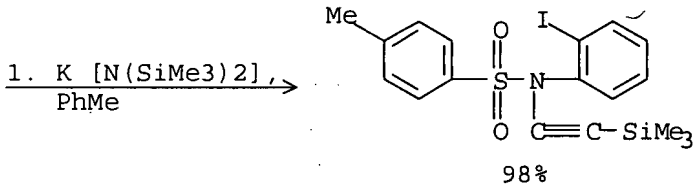
REF: Tetrahedron Letters, 45(4), 817-819; 2004
NOTE: Negishi coupling
CON: STAGE(1) 1.5 hours, reflux
STAGE(2) room temperature

L6 ANSWER 41 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(22) OF 72



(step 1) (step 2) (step 2)



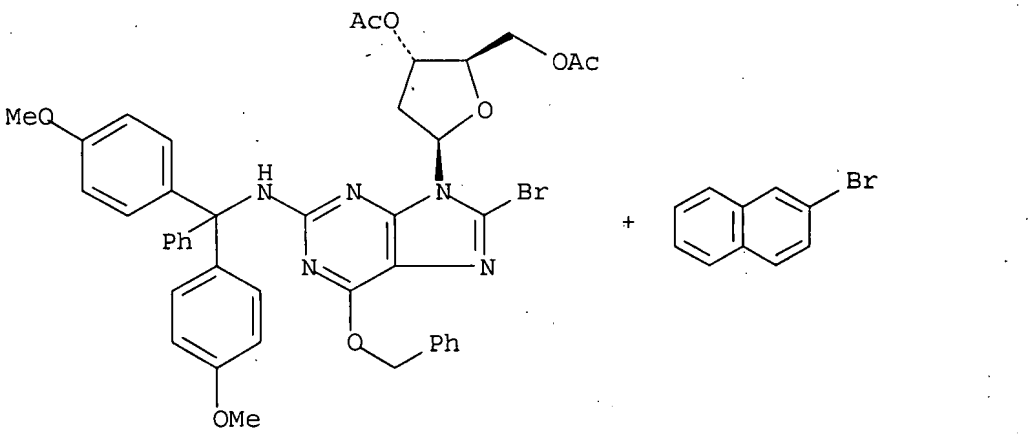
98%

REF: Angewandte Chemie, International Edition, 42(35), 4257-4260; 2003
CON: STAGE(2) room temperature

L6 ANSWER 42 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

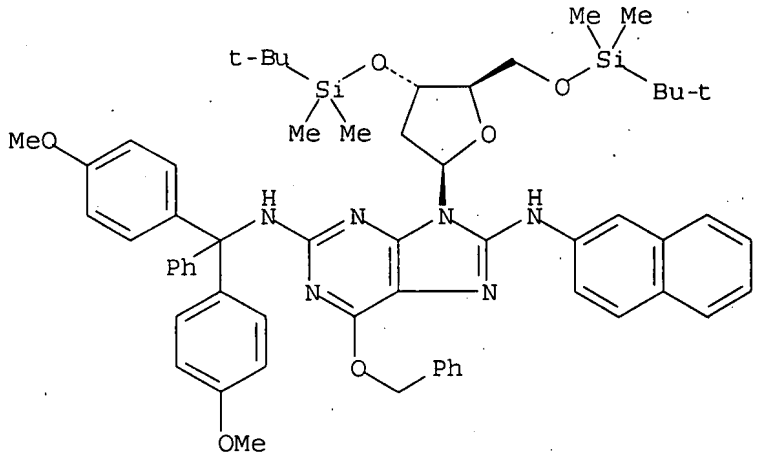
CAS ONLINE PRINTOUT

RX(32) OF 51 - 4 STEPS



3. t-BuSiMe2Cl

RX(32) OF 51 - 4 STEPS

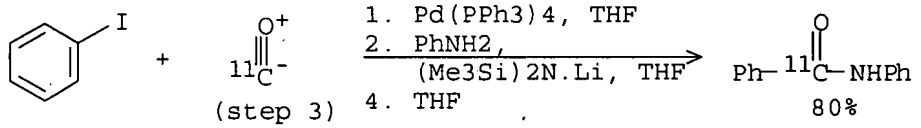


88%

REF: Tetrahedron Letters, 44(32), 5969-5973; 2003
CON: STEP(1.1) 8 hours, 65 deg C; 65 deg C -> room temperature
STEP(2) 0 deg C
STEP(4.1) 2 hours, 100 deg C; 100 deg C -> 25 deg C

L6 ANSWER 43 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(14) OF 30



(step 3)

1. Pd(PPh3)4, THF
2. PhNH2, (Me3Si)2N.Li, THF
4. THF

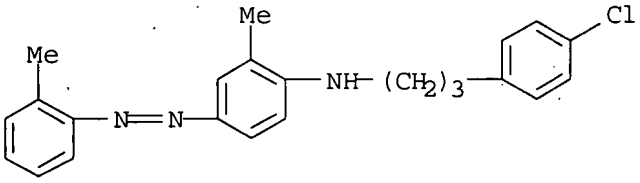
80%

REF: Organic & Biomolecular Chemistry, 1(3), 541-546; 2003
CON: STAGE(1) 1 minute, 70 deg C; 10 - 15 minutes, room temperature
STAGE(2) 10 - 15 minutes, room temperature
STAGE(3) 5 minutes, 150 deg C

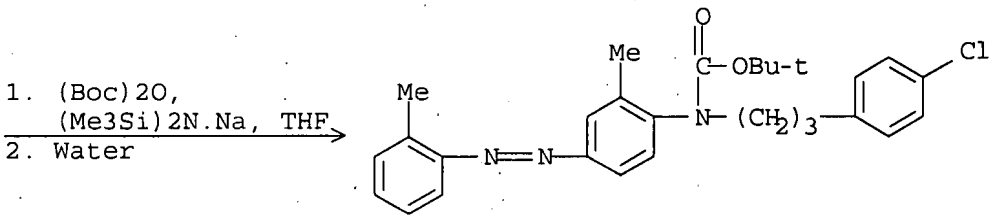
CAS ONLINE PRINTOUT

L6 ANSWER 44 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(7) OF 21



(step 1)

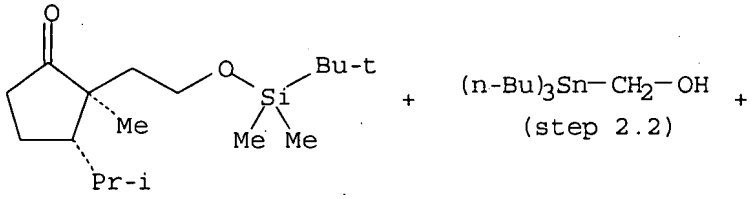


74%

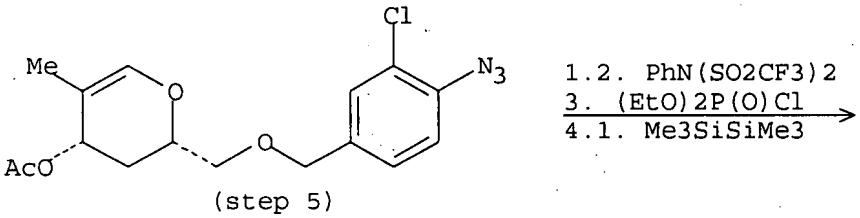
REF: Journal of the American Chemical Society, 125(23), 6977-6985; 2003
CON: 12 hours, 60 deg C

L6 ANSWER 45 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(319) OF 681 - 5 STEPS



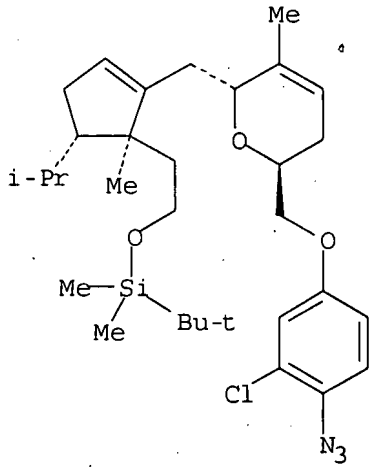
(step 2.2)



(step 5)

CAS ONLINE PRINTOUT

RX(319) OF 681 - 5 STEPS



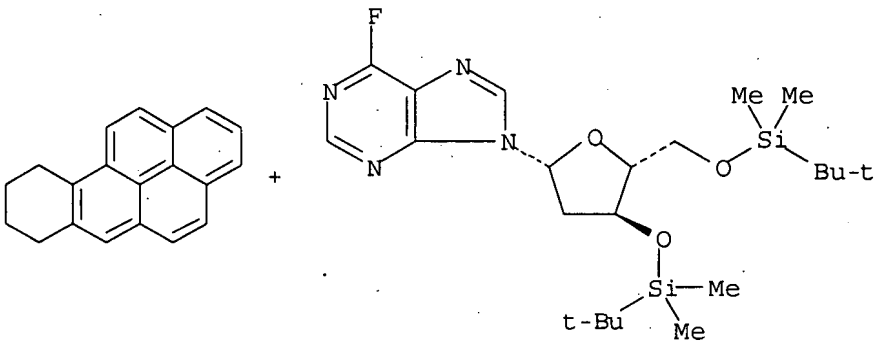
96%

REF: Journal of the American Chemical Society, 125(7), 1843-1850; 2003

NOTE: 2) Stille cross-coupling, 4) stereoselective, 5) stereoselective
CON: STEP(1.1) 1 hour, 0 deg C
STEP(1.2) 4 minutes, 0 deg C; 45 minutes, 0 deg C
STEP(2.1) room temperature -> 70 deg C
STEP(2.2) 8 hours, 70 deg C; 5 hours, 70 deg C
STEP(3.1) 0 deg C; 2 hours
STEP(4.1) 5 minutes, 0 deg C
STEP(4.2) 5 minutes, 0 deg C
STEP(4.3) 0 deg C -> -60 deg C
STEP(4.4) 2 hours, -60 deg C
STEP(4.5) 30 minutes, room temperature
STEP(5) -78 deg C

L6 ANSWER 46 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

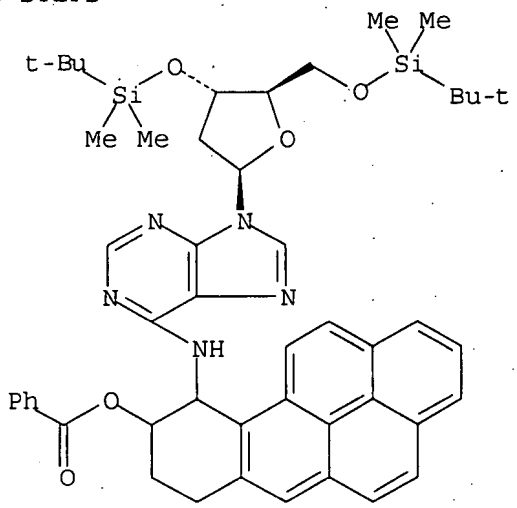
RX(11) OF 13 - 2 STEPS



1.6. Benzoyl cyanide

CAS ONLINE PRINTOUT

RX(11) OF 13 - 2 STEPS



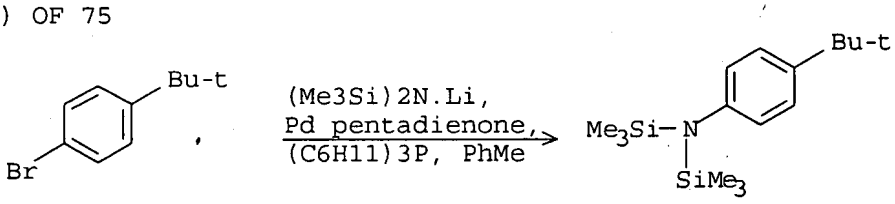
75%

REF: Organic Letters, 5(1), 39-42; 2003

NOTE: 1) stereoselective, 2) stereoselective, isomer mix.
CON: STEP(1.1) 24 hours, room temperature
STEP(1.2) reflux
STEP(1.3) 1 hour, 0 deg C
STEP(1.4) 2.5 hours, 0 deg C
STEP(1.5) 24 hours, 40 deg C
STEP(1.6) 20 minutes, room temperature
STEP(1.7) 2.5 hours, room temperature
STEP(2) 5.5 hours, 90 - 91 deg C

L6 ANSWER 47 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 75



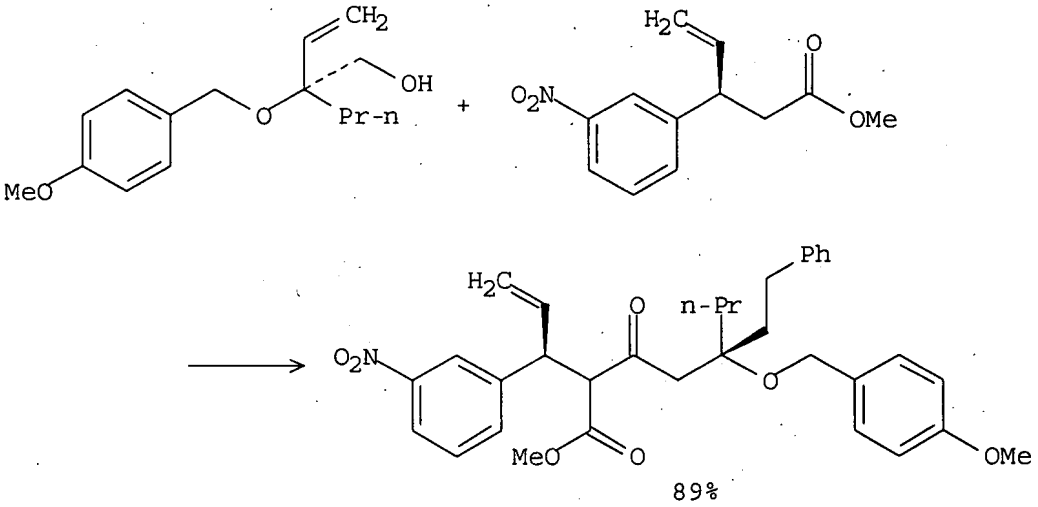
83%

REF: PCT Int. Appl., 2003006420, 23 Jan 2003
NOTE: in-situ generated catalyst, yield depends on temp.
CON: 12 hours, 90 deg C

L6 ANSWER 48 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

CAS ONLINE PRINTOUT

RX(57) OF 149 - 5 STEPS



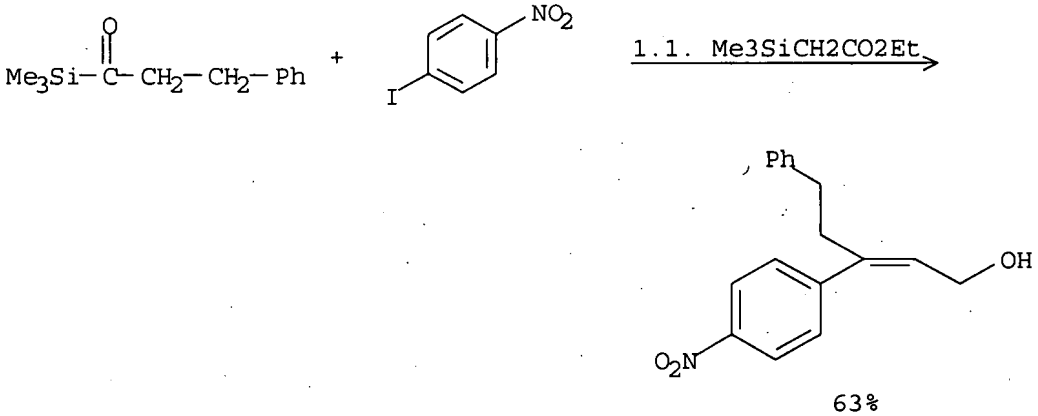
89%

REF: Journal of the American Chemical Society, 124(48), 14320-14321; 2002

NOTE: 1) stereoselective
CON: STEP(1) reflux
STEP(2) reflux; 1 atm
STEP(3.1) 25 deg C
STEP(3.2) reflux
STEP(4.1) 25 deg C
STEP(4.2) 25 deg C
STEP(4.3) 25 deg C
STEP(5.1) -78 deg C
STEP(5.2) -78 deg C
STEP(5.3) 25 deg C

L6 ANSWER 49 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(88) OF 102 - 3 STEPS



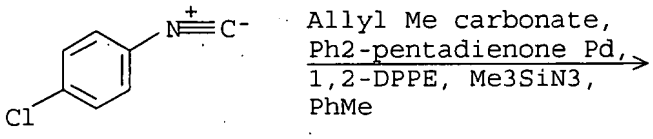
63%

REF: Journal of Organic Chemistry, 67(24), 8450-8456; 2002

NOTE: 1) stereoselective, 2) stereoselective, 3) stereoselective
CON: STEP(1.1) 15 minutes, -78 deg C; -78 deg C -> 0 deg C; 4 hours, 0 deg C
STEP(2.1) 2 hours, room temperature
STEP(2.2) room temperature
STEP(3.1) 20 minutes, room temperature; 2 hours, room temperature
STEP(3.2) room temperature
STEP(3.3) 2 hours, room temperature
STEP(3.4) room temperature

L6 ANSWER 50 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(10) OF 70

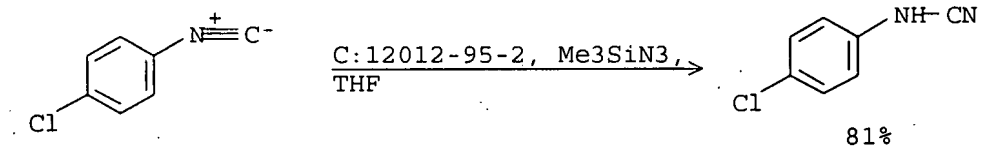


85%

REF: Journal of the American Chemical Society, 124(40), 11940-11945; 2002
NOTE: anaerobic, reaction temp. must be about 40C

L6 ANSWER 51 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(22) OF 50



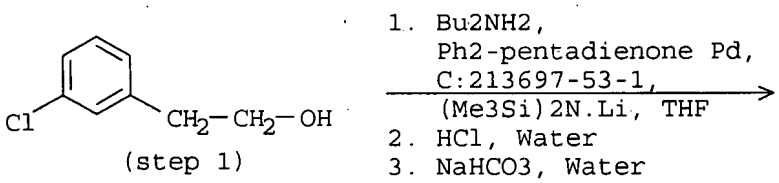
81%

REF: Angewandte Chemie, International Edition, 41(10), 1780-1782; 2002

L6 ANSWER 52 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

CAS ONLINE PRINTOUT

RX(1) OF 19



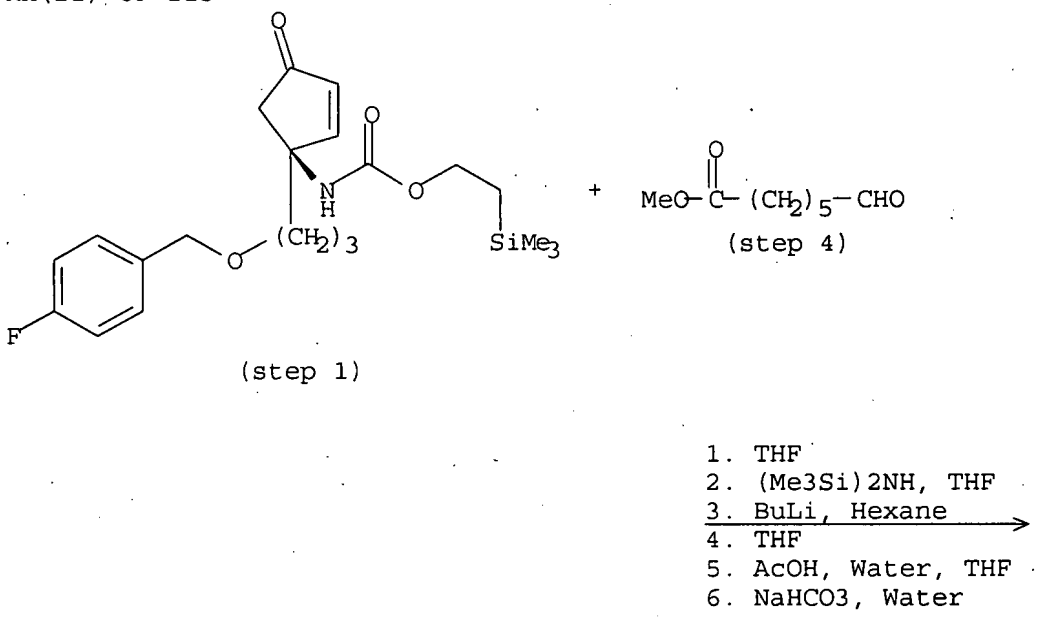
(step 1)

64%

REF: Organic Letters, 4(17), 2885-2888; 2002

L6 ANSWER 53 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(21) OF 213

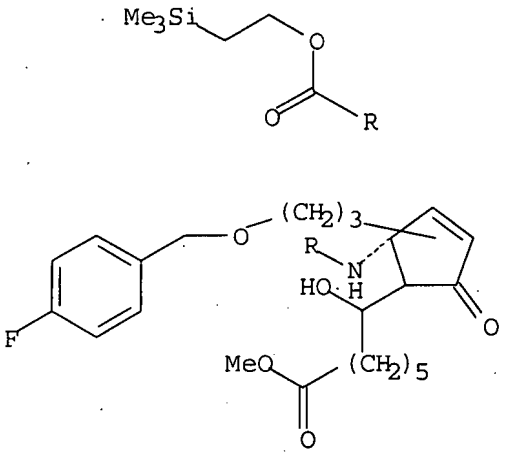


(step 1)

(step 4)

CAS ONLINE PRINTOUT

RX(21) OF 213

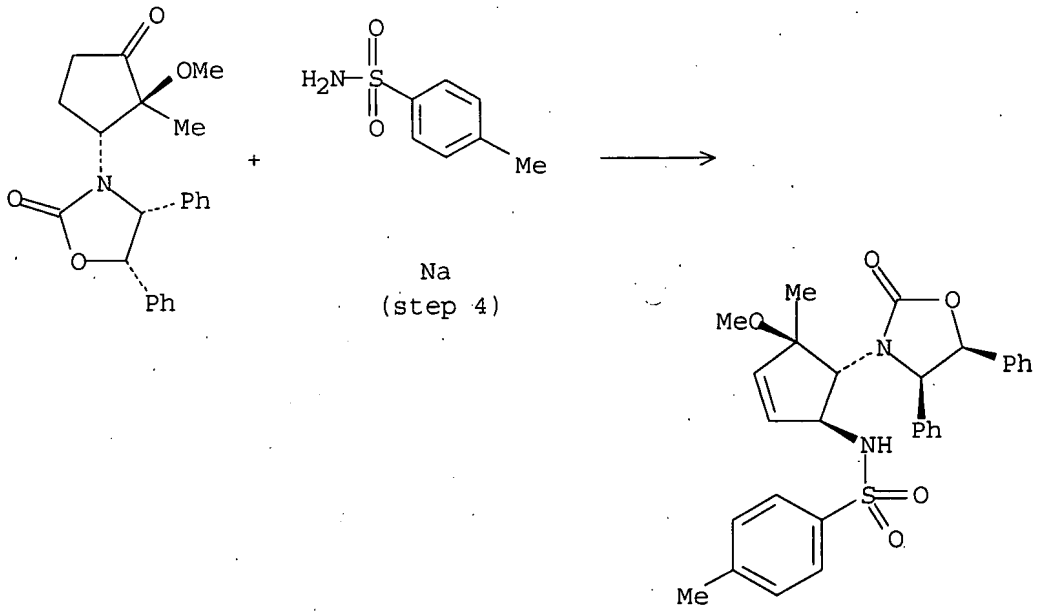


59%

REF: Journal of Organic Chemistry, 67(13), 4399-4406; 2002
NOTE: stereoselective, isomer mix.

L6 ANSWER 54 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(85) OF 113 - 4 STEPS



62%

REF: Journal of Organic Chemistry, 67(11), 3788-3795; 2002
NOTE: 2) stereoselective, 4) stereoselective

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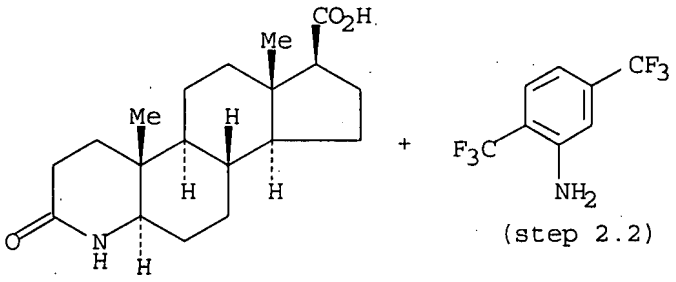
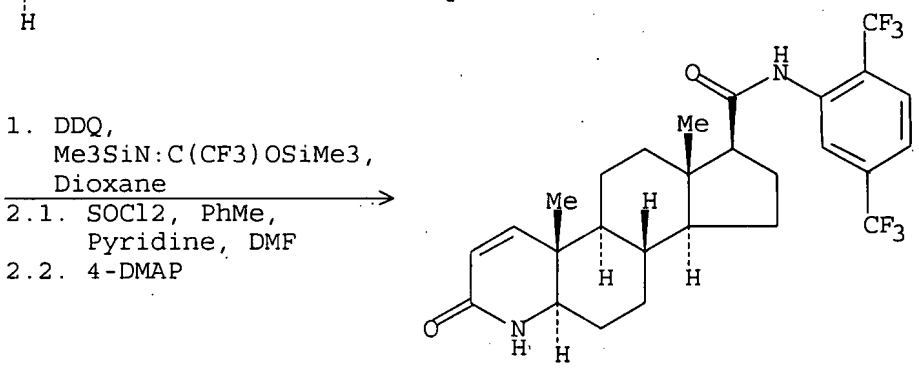
CAS ONLINE PRINTOUT

RX(5) OF 6 - 2 STEPS





94%

REF: PCT Int. Appl., 2002046207, 13 Jun 2002

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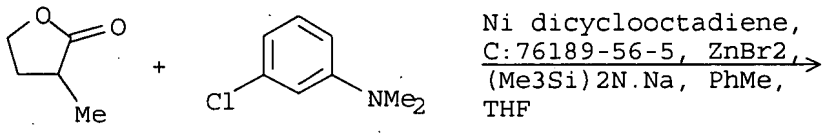
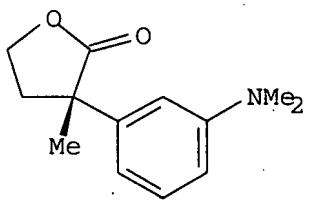
RX(7) OF 22





82%

REF: Journal of the American Chemical Society, 124(14), 3500-3501; 2002
NOTE: stereoselective

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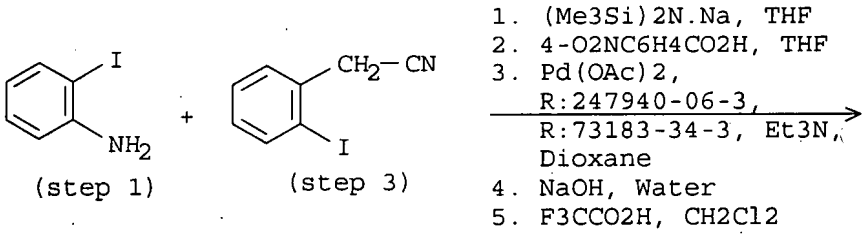
CAS ONLINE PRINTOUT

RX(26) OF 53



REF: Journal of Organic Chemistry, 67(4), 1199-1207; 2002
NOTE: solid-supported reaction, first stage is attachment to Wang resin, alternative preparation shown, Suzuki coupling

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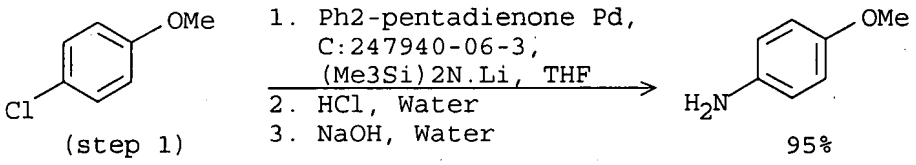
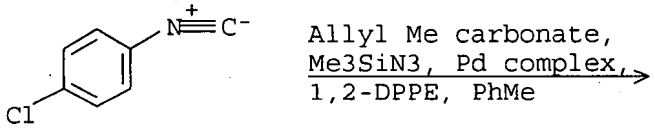
RX(1) OF 18

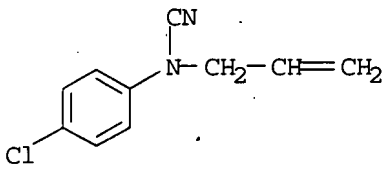


REF: Organic Letters, 3(21), 3417-3419; 2001

L6 ANSWER 59 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(5) OF 10





REF: Journal of the American Chemical Society, 123(38), 9453-9454; 2001

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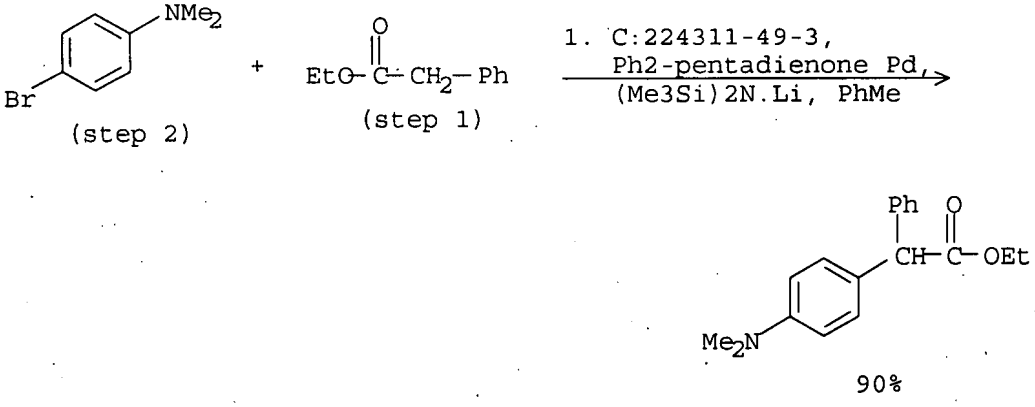
CAS ONLINE PRINTOUT

RX(23) OF 29



REF: Journal of the American Chemical Society, 123(33), 7996-8002; 2001
NOTE: catalyst generated in-situ, alternative reaction conditions gave lower yield

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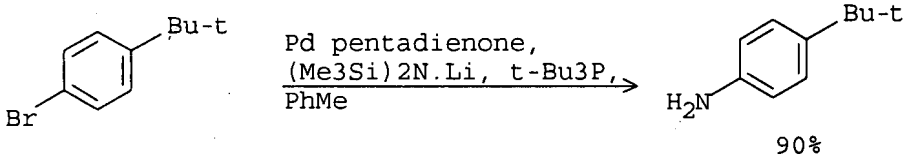
RX(1) OF 23



REF: Organic Letters, 3(17), 2729-2732; 2001

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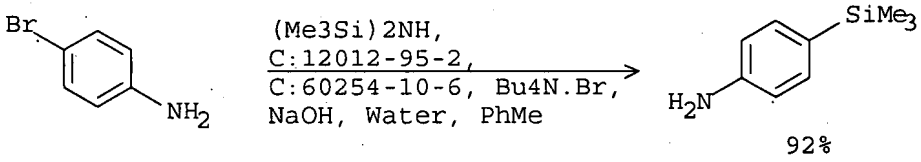
RX(4) OF 14



REF: Chemical Communications (Cambridge), (19), 1895-1896; 2000

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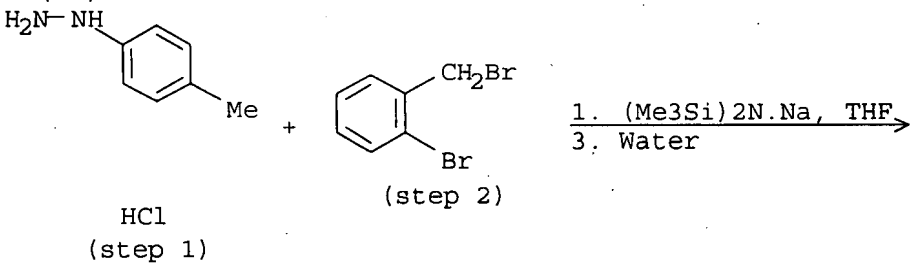
CAS ONLINE PRINTOUT

RX(11) OF 12



REF: Organic Letters, 2(4), 519-521; 2000
NOTE: other reactants similarly prepd.

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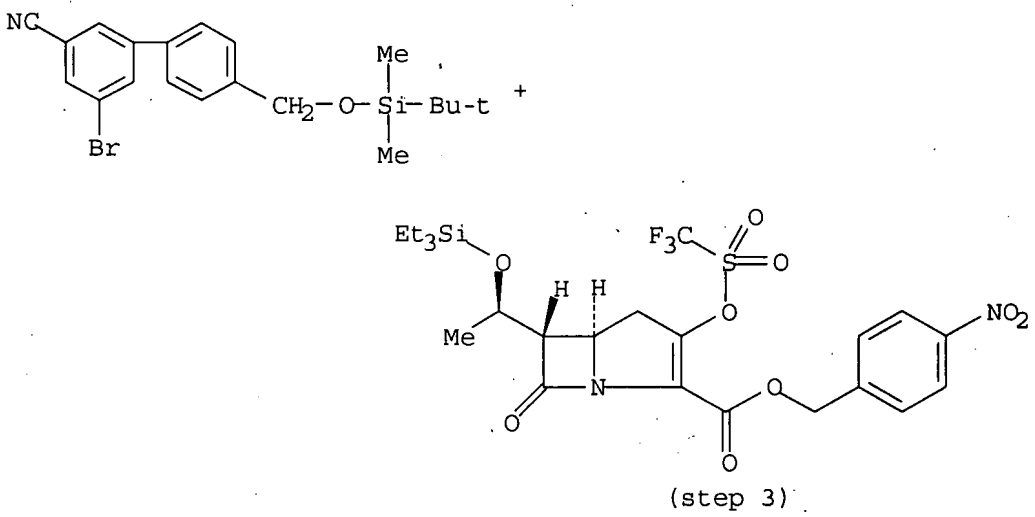
RX(32) OF 50 - 3 STEPS



RX(32) OF 50 - 3 STEPS

1.1. R:5419-55-6, THF, PhMe
1.2. BuLi, Hexane
1.3. H2SO4, Water
2. Me3SiN:CMeOSiMe3, THF
3. Pd pentadienone, KOH, PhMe

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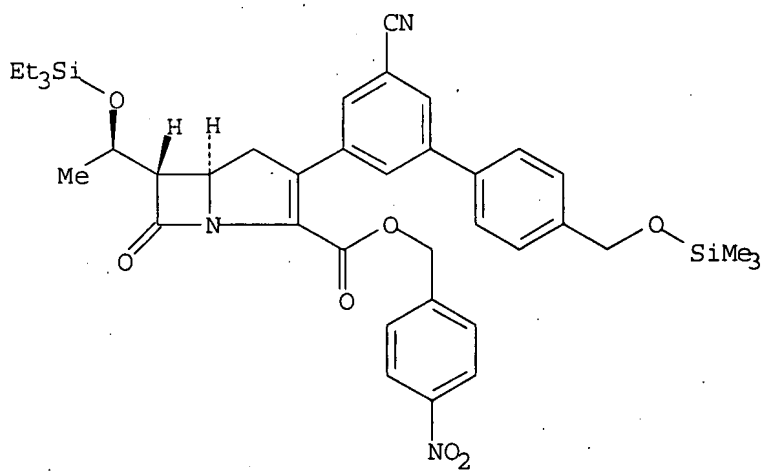
RX(32) OF 50 - 3 STEPS



REF: PCT Int. Appl., 9531461, 23 Nov 1995
NOTE: 3) key step

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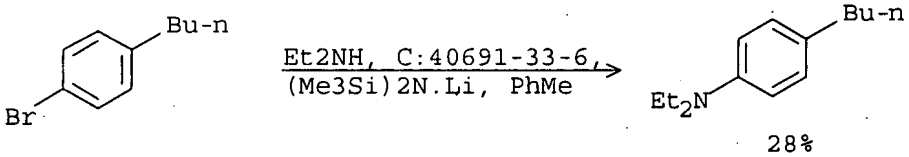
RX(2) OF 4



REF: Tetrahedron Letters, 36(21), 3609-12; 1995

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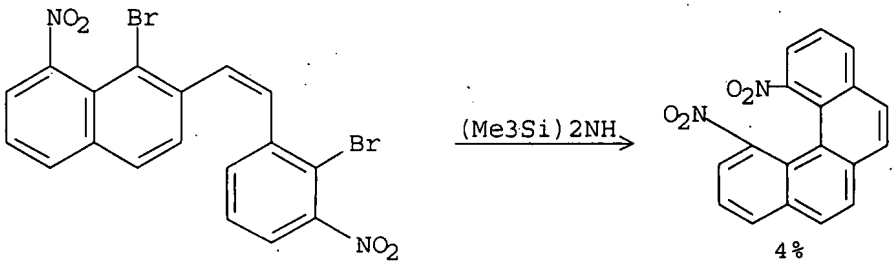
RX(2) OF 7



REF: Tetrahedron Letters, 36(17), 2967-70; 1995
NOTE: TETRAKIS(TRIPHENYLPHOSPHINE)PALLADIUM(0)

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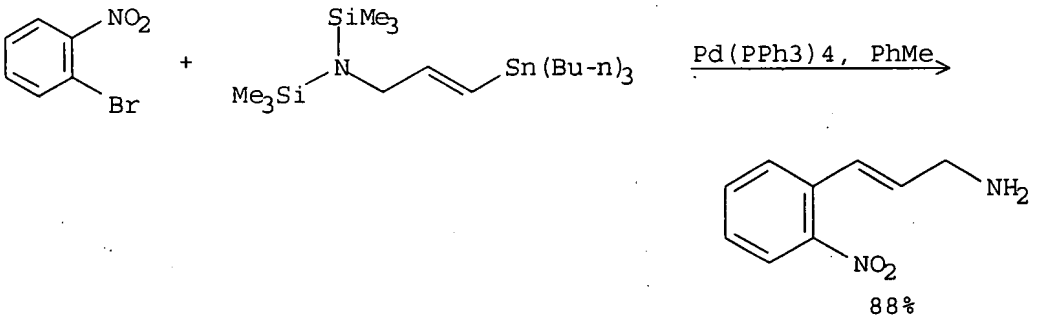
CAS ONLINE PRINTOUT

RX(6) OF 51



88%

REF: Bulletin de la Societe Chimique de France, 130(3), 273-80; 1993
NOTE: stereoselective

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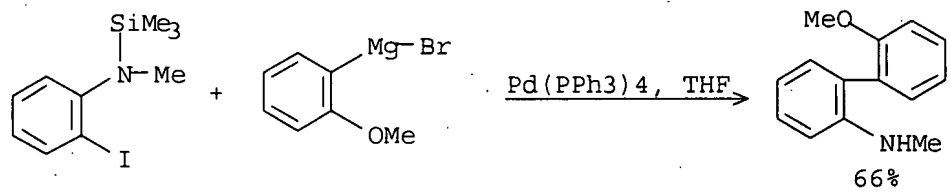
RX(4) OF 12



66%

REF: Tetrahedron, 42(7), 2111-16; 1986

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